

Table S1. ¹H NMR (500 MHz, δ_{H} , multi, (J in Hz) and ¹³C NMR (125 MHz) spectral data of **1** and guttiferone Q

No.	<i>Epi-guttiferone Q (1)</i> (Acetone- d_6)			<i>Guttiferone Q</i> (Methanol- d_4)	
	$\delta_{\text{H}}^{\text{a}}$, J (Hz)	$\delta_{\text{C}}^{\text{a}}$	$\delta_{\text{H}}^{\text{b}}$, J (Hz)	$\delta_{\text{H}}^{\text{b}}$, J (Hz)	$\delta_{\text{C}}^{\text{b}}$
1		196.7			196.6
2		118.5			118.4
3		188.8			188.4
4	3.41 (<i>s</i>)	65.6		3.35 (<i>s</i>)	67.7
5		48.8			48.3
6	1.63 (<i>m</i>)	41.8		1.78 (<i>m</i>)	42.1
7	2.32 (<i>t</i> , $J = 7.5$) 2.01 (<i>m</i>)	43.1		2.06 (<i>dd</i> , $J = 13.2$, 4.0) 1.60 (<i>t</i> , $J = 13.2$)	42.9
8		65.1			64.9
9		208.2			208.0
10		198.7			198.3
11		138.5			139.5
12	7.51 (<i>d</i> , $J = 7.5$)	129.5	7.57 (<i>d</i> , $J = 7.5$)	7.56 (<i>m</i>)	129.7
13	7.43 (<i>t</i> , $J = 7.5$)	128.6	7.38 (<i>t</i> , $J = 7.5$)	7.40 (<i>t</i> , $J = 7.7$)	128.9
14	7.57 (<i>t</i> , $J = 7.5$)	133.1	7.53 (<i>t</i> , $J = 7.5$)	7.54 <i>m</i>	133.3
15	7.43 (<i>t</i> , $J = 7.5$)	128.6	7.38 (<i>t</i> , $J = 7.5$)	7.40 (<i>t</i> , $J = 7.7$)	128.9
16	7.51 (<i>d</i> , $J = 7.5$)	129.5	7.57 (<i>d</i> , $J = 7.5$)	7.56 (<i>m</i>)	129.7
17	1.00 (<i>s</i>)	18.2	0.94 (<i>s</i>)	0.93 (<i>s</i>)	18.4
18	1.70 (<i>m</i>) 1.47 (<i>m</i>)	39.3		1.67 (<i>m</i>) 1.46 (<i>td</i> , $J = 12.8$, 4.1)	39.8
19	2.42 (<i>m</i>) 2.02 (<i>m</i>)	22.7		2.36 (<i>m</i>) 2.06 (<i>m</i>)	23.0
20	5.14 (<i>m</i>)	125.2	5.09 (<i>m</i>)	5.12 (<i>brt</i> , $J = 7.0$)	125.4
21		132.0		–	132.5
22	1.67 (<i>s</i>)	17.8	1.57 (<i>s</i>)	1.66 (<i>s</i>)	18.2
23	1.68 (<i>s</i>)	25.9	1.63 (<i>s</i>)	1.73 (<i>s</i>)	26.0
24	2.20 (<i>m</i>) 1.65 (<i>m</i>)	28.8		2.20 (<i>m</i>) 1.70 (<i>m</i>)	29.1
25	4.99 (<i>m</i>)	123.4	5.01 (<i>m</i>)	5.05 (<i>brt</i> , $J = 6.5$)	123.6
26		133.7		–	134.4
27	1.56 (<i>s</i>)	18.0	1.61 (<i>s</i>)	1.60 (<i>s</i>)	17.8
28	1.63 (<i>s</i>)	25.9	1.67 (<i>s</i>)	1.69 (<i>s</i>)	25.9
29	2.49 (<i>m</i>) 2.34 (<i>m</i>)	31.1		2.42 (<i>m</i>)	31.1
30	5.23 (<i>m</i>)	121.0	5.16 (<i>m</i>)	5.18 (<i>br t</i> , $J = 7.3$)	121.1

31		134.7		–	135.2
32	1.62 (<i>s</i>)	18.1	1.66 (<i>s</i>)	1.65 (<i>s</i>)	18.0
33	1.74 (<i>s</i>)	26.2	1.71 (<i>s</i>)	1.70 (<i>s</i>)	26.2
^a acetone- <i>d</i> ₆ ^b methanol- <i>d</i> ₄					

Table S2. ¹H NMR (500 MHz, δ_H, multi, (*J* in Hz) and ¹³C NMR (125 MHz) data of compounds **1** and **2** in acetone-*d*₆.

No.	1 (acetone- <i>d</i> ₆)		2 (acetone- <i>d</i> ₆)	
	δ _H (ppm), <i>J</i> (Hz)	δ _C (ppm)	δ _H (ppm), <i>J</i> (Hz)	δ _C (ppm)
1	–	196.7	–	206.3
2	–	118.5	–	69.9
3	–	188.8	–	43.4
4	3.41 (<i>s</i>)	65.6	–	43.3
5	–	48.8	–	43.1
6	1.63 (<i>m</i>)	41.8	–	62.8
7	2.32 (<i>t</i> , <i>J</i> = 7.5) 2.01 (<i>m</i>)	43.1	–	195.2
8	–	65.1	–	121.0
9	–	208.2	–	191.8
10	–	198.7	2.76 (<i>m</i> , 1H) 2.57 (<i>m</i> , 1H)	26.2
11	–	138.5	4.92 (<i>m</i> , 1H)	121.0
12	7.51 (<i>d</i> , <i>J</i> = 7.5)	129.5	–	134.9
13	7.43 (<i>t</i> , <i>J</i> = 7.5)	128.6	1.64 (<i>s</i> , 3H)	18.2
14	7.57 (<i>t</i> , <i>J</i> = 7.5)	133.1	1.64 (<i>s</i> , 3H)	26.2
15	7.43 (<i>t</i> , <i>J</i> = 7.5)	128.6	0.86 (<i>s</i> , 3H)	14.3
16	7.51 (<i>d</i> , <i>J</i> = 7.5)	129.5	–	37.1
17	1.00 (<i>s</i>)	18.2	–	24.5
18	1.70 (<i>m</i>) 1.47 (<i>m</i>)	39.3	4.99 (<i>s</i> , 1H)	125.2
19	2.42 (<i>m</i>) 2.02 (<i>m</i>)	22.7	–	133.0
20	5.14 (<i>br s</i>)	125.2	1.70 (<i>s</i> , 3H)	17.8
21	–	132.0	1.56 (<i>s</i> , 3H)	25.6
22	1.67 (<i>s</i>)	17.8	–	30.4
23	1.68 (<i>s</i>)	25.9	5.08 (<i>m</i> , 1H)	123.5
24	2.20 (<i>m</i>) 1.65 (<i>m</i>)	28.8	–	132.1

25	4.99 (<i>br s</i>)	123.4	1.69 (<i>s</i> , 3H)	25.8
26	–	133.7	1.59 (<i>s</i> , 3H)	18.1
27	1.56 (<i>s</i>)	18.0	–	198.6
28	1.63 (<i>s</i>)	25.9	–	138.3
29	2.49 (<i>m</i>) 2.34 (<i>m</i>)	31.1	7.51 (<i>d</i> , $J = 7.5$, 1H)	130.5
30	5.23 (<i>br s</i>)	121.0	7.42 (<i>t</i> , $J = 7.5$, 1H)	129.6
31	–	134.7	7.57 (<i>t</i> , $J = 7.5$, 1H)	133.3
32	1.62 (<i>s</i>)	18.1	7.42 (<i>t</i> , $J = 7.5$, 1H)	129.6
33	1.74 (<i>s</i>)	26.2	7.51 (<i>d</i> , $J = 7.5$, 1H)	130.5

Table S3. ^1H NMR (500 MHz, δ_{H} , multi, (J in Hz) and ^{13}C NMR (125 MHz) spectral data comparison of compound **3** in acetone- d_6 .

No.	3 (acetone- d_6)		Guttiferone K (methanol- d_4)	
	δ_{H} (ppm), J (Hz)	δ_{C} (ppm)	δ_{H} (ppm), J (Hz)	δ_{C} (ppm)
1	–	196.9	–	196.7
2	–	117.8	–	119.9
3	–	191.9	–	191.0
4	–	68.0	–	69.4
5	–	51.3	–	51.6
6	1.60 (<i>m</i>)	40.3	1.75 (<i>m</i>)	42.0
7	2.07 (<i>m</i>) 1.44 (<i>m</i>)	42.8	2.03 (<i>dd</i> , $J = 13.3$, 3.3) 1.44 (<i>dd</i> , $J = 13.3$, 3.3)	43.2
8	–	65.1	–	64.1
9	–	207.9	–	209.2
10	–	196.5	–	196.7
11	–	129.8	–	130.3
12	7.19 (<i>d</i> , $J = 2.0$)	117.4	7.20 (<i>d</i> , $J = 2.1$)	117.4
13	–	151.3	–	146.5
14	–	145.4	–	152.6
15	6.80 (<i>d</i> , $J = 8.0$)	114.9	6.69 (<i>d</i> , $J = 8.4$)	115.3
16	7.01 (<i>dd</i> , $J = 8.5$, 2.0)	124.6	6.95 (<i>dd</i> , $J = 8.4$, 2.1)	125.1
17	2.79 (<i>dd</i> , $J = 14.5$, 8.5) 2.68 (<i>m</i>)	26.5	2.73 (<i>dd</i> , $J = 13.0$, 7.8) 2.65 (<i>dd</i> , $J = 13.0$, 4.3)	26.7
18	4.92 (<i>m</i>)	121.4	4.88 (<i>m</i>)	121.5
19	–	134.2	–	135.2
20	1.70 (<i>s</i>)	18.3	1.69 (<i>s</i>)	18.5
21	1.66 (<i>s</i>)	25.9	1.62 (<i>s</i>)	26.4
22	0.86 (<i>s</i>)	17.8	0.81 (<i>s</i>)	16.4

23	1.81 (<i>m</i>) 1.77 (<i>m</i>)	36.9	1.68 (<i>m</i>)	37.6
24	2.12 (<i>m</i>) 1.99 (<i>m</i>)	25.0	2.07 (<i>m</i>) 1.77 (<i>m</i>)	30.2
25	5.01 (<i>br t</i> , <i>J</i> = 6.8)	125.4	5.00 (<i>br t</i> , <i>J</i> = 7.0)	123.7
26	–	131.9	–	134.7
27	1.66 (<i>s</i>)	18.2	1.67 (<i>s</i>)	18.3
28	1.60 (<i>s</i>)	25.9	1.57 (<i>s</i>)	26.0
29	2.55 (<i>m</i>) 2.45 (<i>m</i>)	31.4	2.51 (<i>dd</i> , <i>J</i> = 14.5, 8.8) 2.44, (<i>dd</i> , <i>J</i> = 14.5, 8.8)	31.8
30	5.09 (<i>br t</i> , <i>J</i> = 6.0)	120.9	5.10 (<i>br t</i> , <i>J</i> = 7.1)	121.1
31	–	134.7	–	135.7
32	1.67 (<i>s</i>)	18.1	1.67 (<i>s</i>)	18.4
33	1.70 (<i>s</i>)	26.2	1.71 (<i>s</i>)	26.4
34	1.99 (<i>m</i>)	26.4	1.97 (<i>m</i>)	25.3
35	5.18 (<i>br t</i> , <i>J</i> = 7.0)	123.5	5.04 (<i>br t</i> , <i>J</i> = 6.9)	125.6
36	–	133.8	–	132.7
37	1.66 (<i>s</i>)	25.9	1.66 (<i>s</i>)	26.1
38	1.57 (<i>s</i>)	18.1	1.59 (<i>s</i>)	18.0

Table S4. ¹H NMR (500 MHz, δ_H, multi, (*J* in Hz) and ¹³C NMR (125 MHz) data of compound **4** in acetone-*d*₆.

No.	4 (acetone- <i>d</i> ₆)		Hypersampsonse I (pyridine- <i>d</i> ₅)	
	δ _H (ppm), <i>J</i> (Hz)	δ _C (ppm)	δ _H (ppm), <i>J</i> (Hz)	δ _C (ppm)
1	–	81.3	–	81.9
2	–	206.1	–	205.8
3	–	70.8	–	76.6
4 α	2.52 (<i>m</i>)	29.2	2.72 (<i>m</i>)	29.0
4 β	2.32 (<i>m</i>)		2.56 (<i>ddd</i> , <i>J</i> = 14.1, 9.4, 3.9)	
5 α	1.82 (<i>m</i>)	42.2	1.78 (over load)	41.8
5 β			2.00 (<i>m</i>)	
6	–	44.6	–	44.3
7	2.09 (<i>m</i>)	58.3	2.20 (<i>m</i>)	58.0
8 α	2.32 (<i>m</i>)	29.3	2.25 (<i>m</i>)	28.9
8 β	1.80 (<i>m</i>)		1.55 (over load)	
9	2.40 (<i>m</i>)	43.9	2.14 (<i>m</i>)	43.5
10a	2.63 (<i>m</i>)	45.2	2.65 (<i>dd</i> , <i>J</i> = 13.9, 6.1)	45.1

10b	1.99 (<i>m</i>)		1.98 (<i>m</i>)	
11	–	69.3	–	69.1
12	–	206.4	–	206.1
13	–	51.2	–	51.9
14	–	206.1	–	205.9
15	–	193.4	–	193.7
16	–	134.7	–	135.6
17	7.18 (<i>d</i> , <i>J</i> = 8.0)	129.8	7.54 (<i>br d</i> , <i>J</i> = 7.8)	129.8
18	7.36 (<i>dd</i> , <i>J</i> = 16.0, 8.0)	128.7	7.37 (<i>m</i>)	128.5
19	7.47 (<i>t</i> , <i>J</i> = 7.0)	132.7	7.40 (<i>m</i>)	132.5
20	7.36 (<i>dd</i> , <i>J</i> = 16.0, 8.0)	128.7	7.37 (<i>m</i>)	128.5
21	7.18 (<i>d</i> , <i>J</i> = 8.0)	129.8	7.54 (<i>br d</i> , <i>J</i> = 7.8)	129.8
22	0.92 (<i>s</i>)	22.0	0.95 (<i>s</i>)	21.8
23	1.03 (<i>s</i>)	30.3	0.92 (<i>s</i>)	29.9
24a	2.63 (<i>m</i>)	30.4	2.86 (<i>dd</i> , <i>J</i> = 14.5, 7.8)	30.4
24b	2.53 (<i>m</i>)		2.74 (<i>m</i>)	
25	5.16 (<i>m</i>)	120.5	5.42 (<i>t</i> , <i>J</i> = 6.5)	120.2
26	–	138.2	–	138.1
27	2.07 (<i>m</i>)	40.6	2.07 (<i>m</i>)	40.3
28	1.68 (<i>s</i>)	16.5	1.77 (<i>s</i>)	16.6
29	2.07 (<i>m</i>)	27.2	2.12 (<i>m</i>)	26.9
30	5.08 (<i>d</i> , <i>J</i> = 7.5)	124.9	5.17 (<i>br t</i> , <i>J</i> = 7.4)	124.6
31	–	132.0	–	131.4
32	1.64 (<i>s</i>)	25.4	1.66 (<i>s</i>)	25.8
33	1.58 (<i>s</i>)	17.7	1.56 (<i>s</i>)	17.7
34	1.44 (<i>s</i>)	25.4	1.58 (<i>s</i>)	25.7
35	1.48 (<i>s</i>)	22.8	1.62 (<i>s</i>)	22.8

Table S5. ¹H NMR (400 MHz, δ_H, multi, (*J* in Hz) and ¹³C NMR (100 MHz) spectral data comparison of compound **5** in CDCl₃.

No.	5 (CDCl ₃)		Sampsonione D (CDCl ₃)	
	δ _H (ppm), <i>J</i> (Hz)	δ _C (ppm)	δ _H (ppm), <i>J</i> (Hz)	δ _C (ppm)
1	–	80.8	–	80.8
2	–	203.8	–	203.9
3	–	73.9	–	73.9
4α	2.64 (1H, <i>m</i>)	34.3	2.63 (1H, <i>t</i> , <i>J</i> = 12.6)	34.4
4β	2.06 (1H, <i>m</i>)		2.08 (1H, <i>dd</i> , <i>J</i> = 12.4, 8.8)	
5β	3.15 (1H, <i>m</i>)	54.9	3.12 (1H, <i>dd</i> , <i>J</i> = 12.0, 8.9)	54.9
6	–	44.2	–	44.3
7α	2.03 (1H, <i>m</i>)	57.1	2.03 (1H, <i>m</i>)	57.2

8 α	2.29 (1H, <i>m</i>)	28.8	2.28 (1H, <i>m</i>)	28.9
8 β	1.71 (1H, <i>m</i>)		1.71 (1H, <i>m</i>)	
9 α	2.10-2.12 (1H, <i>m</i>)	43.8	2.13 (1H, <i>m</i>)	43.9
10a	2.52 (1H, <i>m</i>)	42.5	2.52 (1H, <i>dd</i> , <i>J</i> = 14.0, 8.6)	42.6
10b	1.89 (1H, <i>m</i>)		1.88 (1H, <i>d</i> , <i>J</i> = 14.1)	
11	–	68.8	–	68.9
12	–	204.7	–	204.7
13	–	50.6	–	50.7
14	–	206.2	–	206.2
15	–	192.4	–	192.4
16	–	134.8	–	134.8
17	7.12 (1H, <i>d</i> , <i>J</i> = 8.0)	128.8	7.11 (1H, <i>d</i> , <i>J</i> = 7.7)	128.8
18	7.26 (1H, <i>t</i> , <i>J</i> = 7.8)	127.9	7.26 (1H, <i>t</i> , <i>J</i> = 7.9)	127.9
19	7.39 (1H, <i>t</i> , <i>J</i> = 7.4)	131.9	7.39 (1H, <i>t</i> , <i>J</i> = 7.7)	131.3
20	7.26 (1H, <i>t</i> , <i>J</i> = 7.8)	127.9	7.26 (1H, <i>t</i> , <i>J</i> = 7.9)	127.9
21	7.12 (1H, <i>d</i> , <i>J</i> = 8.0)	128.8	7.11 (1H, <i>d</i> , <i>J</i> = 7.7)	128.8
22	–	145.2	–	145.2
23	4.91 (1H, <i>s</i>)	111.7	4.91 (1H, <i>s</i>)	111.8
	4.84 (1H, <i>s</i>)		4.84 (1H, <i>s</i>)	
24	1.80 (3H, <i>s</i>)	23.7	1.80 (3H, <i>s</i>)	23.8
25	0.87 (3H, <i>s</i>)	26.7	0.86 (3H, <i>s</i>)	26.7
26	0.93 (3H, <i>s</i>)	27.0	0.93 (3H, <i>s</i>)	27.0
27	2.16 (2H, <i>m</i>)	29.3	nd	29.3
28	5.11 (1H, <i>t</i> , <i>J</i> = 7.0)	118.9	5.11 (1H, <i>t</i> , <i>J</i> = 5.7)	118.9
29	–	138.2	–	138.3
30	1.95 (2H, <i>m</i>)	39.8	1.98 (2H, <i>m</i>)	39.5
31	1.66 (3H, <i>s</i>)	16.3	1.66 (3H, <i>s</i>)	16.3
32	2.03 (2H, <i>m</i>)	26.5	2.03 (2H, <i>m</i>)	26.5
33	5.05 (1H, <i>t</i> , <i>J</i> = 6.8)	124.0	5.05 (1H, <i>t</i> , <i>J</i> = 4.3)	124.0
34	–	131.2	–	131.3
35	1.65 (3H, <i>s</i>)	25.6	1.65 (3H, <i>s</i>)	25.6
36	1.57 (3H, <i>s</i>)	17.5	1.57 (3H, <i>s</i>)	17.6
37	1.41 (3H, <i>s</i>)	22.7	1.40 (3H, <i>s</i>)	22.7
38	1.46 (3H, <i>s</i>)	25.1	1.46 (3H, <i>s</i>)	25.2

Table S6. ^1H NMR (400 MHz, δ_{H} , multi, (*J* in Hz) and ^{13}C NMR (100 MHz) data of compound **6** in CDCl_3 .

No.	6 (CDCl ₃)		Sampsonione H (CDCl ₃)	
	δ_{H} (ppm), J (Hz)	δ_{C} (ppm)	δ_{H} (ppm), J (Hz)	δ_{C} (ppm)
1	–	79.7	–	81.1
2	–	203.8	–	203.3
3	–	75.1	–	74.8
4 α	2.37 (<i>dd</i> , $J = 11.4, 7.6$)	28.2	2.37 (<i>dd</i> , $J = 13.7, 6.7$)	27.9
4 β	2.43 (<i>m</i>)		2.43 (<i>dd</i> , $J = 13.7, 7.0$)	
5 α	1.75 (<i>m</i>)	42.7	1.72 (<i>m</i>)	42.4
5 β	1.75 (<i>m</i>)		1.72 (<i>m</i>)	
6	–	44.5	–	44.2
7	1.95 (<i>m</i>)	55.6	1.92 (<i>m</i>)	55.3
8 α	1.92 (<i>m</i>)	23.8	1.92 (<i>m</i>)	23.5
8 β	1.75 (<i>m</i>)		1.72 (<i>m</i>)	
9	2.10 (<i>m</i>)	42.5	2.07 (<i>m</i>)	42.2
10a	2.50 (<i>dd</i> , $J = 10.8, 7.2$)	35.3	2.50 (<i>dd</i> , $J = 14.4, 5.3$)	35.0
10b	2.21 (<i>d</i> , $J = 16.4$)		2.21 (<i>d</i> , $J = 14.8$)	
11	–	67.7	–	67.5
12	–	207.5	–	204.8
13	–	47.8	–	47.5
14	–	203.8	–	203.3
15	–	193.4	–	192.9
16	–	135.2	–	134.8
17	7.06 (<i>d</i> , $J = 7.2$)	128.7	7.10 (<i>d</i> , $J = 8.0$)	128.4
18	7.26 (<i>dd</i> , $J = 12.4, 8.8$)	128.4	7.27 (<i>dd</i> , $J = 7.9, 7.0$)	128.1
19	7.38 (<i>t</i> , $J = 7.6$)	132.3	7.39 (<i>t</i> , $J = 7.0$)	132.1
20	7.26 (<i>dd</i> , $J = 12.4, 8.8$)	128.4	7.27 (<i>dd</i> , $J = 7.9, 7.0$)	128.1
21	7.06 (<i>d</i> , $J = 7.2$)	128.7	7.10 (<i>d</i> , $J = 8.0$)	128.4
22	1.01 (<i>s</i>)	28.6	1.03 (<i>s</i>)	28.3
23	0.94 (<i>s</i>)	20.7	0.95 (<i>s</i>)	20.5
24a	2.61 (<i>m</i>)	29.1	2.62 (<i>m</i>)	28.9
24b	2.61 (<i>m</i>)		2.62 (<i>m</i>)	
25	5.30 (<i>t</i> , $J = 8.0$)	119.2	5.30 (<i>t</i> , $J = 7.4$)	118.9
26	–	139.1	–	138.8
27	2.07 (<i>m</i>)	40.2	2.06 (<i>m</i>)	39.9
28	1.66 (<i>s</i>)	16.5	1.67 (<i>s</i>)	16.2
29	2.07 (<i>m</i>)	26.7	2.07 (<i>m</i>)	26.5
30	5.06 (<i>br s</i>)	124.4	5.07 (<i>br s</i>)	124.1
31	–	131.8	–	131.3
32	1.66 (<i>s</i>)	25.9	1.67 (<i>s</i>)	25.7
33	1.59 (<i>s</i>)	17.8	1.58 (<i>s</i>)	17.6
34	1.42 (<i>s</i>)	25.2	1.42 (<i>s</i>)	25.2
35	1.39 (<i>s</i>)	22.6	1.39 (<i>s</i>)	22.5

Table S7. ^1H NMR (500 MHz, δ_{H} , multi, (J in Hz) and ^{13}C NMR (125 MHz) data of compound **7** in acetone- d_6 .

No.	7 (acetone- d_6)		β-Mangostin (acetone- d_6)	
	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)
1	–	160.7	–	159.7
2	–	111.9	–	111.4
3	–	164.6	–	163.5
4	6.52 (1H, <i>s</i>)	89.9	6.33 (1H, <i>s</i>)	88.8
4a	–	155.6	–	155.6
5	6.87 (1H, <i>s</i>)	102.7	6.82 (1H, <i>s</i>)	101.5
6	–	156.3	–	154.4
7	–	144.6	–	142.5
8	–	138.1	–	137.0
8a	–	112.8	–	112.3
9	–	182.9	–	181.9
9a	–	103.7	–	103.7
10a	–	157.8	–	155.2
11	3.32 (2H, <i>d</i> , $J = 6.6$)	21.9	3.36 (2H, <i>d</i> , $J = 6.8$)	21.3
12	5.21 (1H, <i>t</i> , $J = 6.6$)	123.3	5.29 (1H, <i>t</i> , $J = 6.8$)	122.3
13	–	132.0	–	132.0
14	1.63 (3H, <i>s</i>)	25.9	1.85 (3H, <i>s</i>)	25.8
15	1.77 (3H, <i>s</i>)	17.8	1.82 (3H, <i>s</i>)	25.8
16	4.13 (2H, <i>d</i> , $J = 6.6$)	26.9	4.11 (2H, <i>d</i> , $J = 6.8$)	26.5
17	5.27 (1H, <i>t</i> , $J = 6.6$)	124.7	5.25 (1H, <i>t</i> , $J = 6.8$)	123.2
18	–	131.5	–	131.7
19	1.65 (3H, <i>s</i>)	25.9	1.72 (3H, <i>s</i>)	18.2
20	1.83 (3H, <i>s</i>)	18.3	1.71 (3H, <i>s</i>)	17.7
1-OH	13.67 (1H, <i>s</i>)	–	13.44 (1H, <i>s</i>)	–
6-OH	–	–	6.43 (1H, <i>s</i>)	–
3-OMe	3.97 (3H, <i>s</i>)	56.6	3.82 (3H, <i>s</i>)	55.8
7-OMe	3.80 (3H, <i>s</i>)	61.3	3.92 (3H, <i>s</i>)	62.0

Table S8. ^1H NMR (500 MHz, δ_{H} , multi, (J in Hz) and ^{13}C NMR (125 MHz) data of compound **8** in CDCl_3 .

No.	8 (CDCl_3)		α-Mangostin (CDCl_3)	
	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)
1	–	160.7	–	160.6
2	–	108.7	–	108.5

No.	8 (CDCl ₃)		α-Mangostin (CDCl ₃)	
	δ_{H} (ppm) <i>J</i> (Hz)	δ_{C} (ppm)	δ_{H} (ppm) <i>J</i> (Hz)	δ_{C} (ppm)
3	–	161.8	–	161.6
4	6.30 (1H, <i>s</i>)	93.5	6.36 (1H, <i>s</i>)	93.3
4a	–	154.7	–	154.5
5	6.83 (1H, <i>s</i>)	103.7	6.82 (1H, <i>s</i>)	102.8
6	–	155.9	–	155.8
7	–	142.7	–	142.5
8	–	137.2	–	137.0
8a	–	112.3	–	112.2
9	–	182.1	–	182.0
9a	–	101.7	–	101.6
10a	–	155.2	–	155.3
11	3.44 (2H, <i>d</i> , <i>J</i> = 7)	21.6	3.45 (2H, <i>d</i> , <i>J</i> = 6.6)	21.4
12	5.28 (1H, <i>t</i> , <i>J</i> = 7)	121.6	5.29 (1H, <i>t</i> , <i>J</i> = 6.6)	121.5
13	–	132.3	–	131.1
14	1.84 (3H, <i>s</i>)	18.4	1.84 (3H, <i>s</i>)	18.2
15	1.83 (3H, <i>s</i>)	26.0	1.83 (3H, <i>s</i>)	25.8
16	4.08 (2H, <i>d</i> , <i>J</i> = 6.5)	26.7	4.09 (2H, <i>d</i> , <i>J</i> = 6.6)	26.6
17	5.26 (1H, <i>t</i> , <i>J</i> = 6.5)	123.3	5.26 (1H, <i>t</i> , <i>J</i> = 6.6)	123.1
18	–	135.8	–	135.6
19	1.77 (3H, <i>s</i>)	18.1	1.77 (3H, <i>s</i>)	17.9
20	1.69 (3H, <i>s</i>)	26.0	1.69 (3H, <i>s</i>)	25.8
1-OH	–	–	13.78 (1H, <i>s</i>)	–
7-OCH ₃	3.80 (3H, <i>s</i>)	62.2	3.79 (3H, <i>s</i>)	62.0

Table S9. ¹H NMR (500 MHz, δ_{H} , multi, (*J* in Hz) and ¹³C NMR (125 MHz) data of compound **9** in acetone-*d*₆.

No.	9 (acetone- <i>d</i> ₆)		9-Hydroxycalabaxanthone (CDCl ₃)	
	δ_{H} (ppm) <i>J</i> (Hz)	δ_{C} (ppm)	δ_{H} (ppm) <i>J</i> (Hz)	δ_{C} (ppm)
1	–	158.8	–	157.8
2	–	105.2	–	104.4
3	–	160.7	–	nd
4	6.26 (1H, <i>s</i>)	94.6	6.24 (1H, <i>s</i>)	94.0
4a	–	157.2	–	156.1
5	6.87 (1H, <i>s</i>)	102.9	6.83 (1H, <i>s</i>)	101.6
6	–	158.8	–	154.5

No.	9 (acetone- d_6)		9-Hydroxycalabaxanthone (CDCl ₃)	
	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)
7	–	144.8	–	142.7
8	–	138.2	–	136.9
8a	–	111.8	–	112.1
9	–	183.1	–	181.8
9a	–	104.5	–	103.6
10	–	–	–	–
10a	–	157.2	–	155.6
11	6.68 (1H, <i>d</i> , $J = 10.0$)	116.0	6.73 (1H, <i>d</i> , $J = 9.9$)	115.6
12	5.72 (1H, <i>d</i> , $J = 10.0$)	125.5	5.57 (1H, <i>d</i> , $J = 9.9$)	126.9
13	–	78.8	–	77.8
14	1.46 (3H, <i>s</i>)	28.5	1.46 (3H, <i>s</i>)	28.3
15	1.46 (3H, <i>s</i>)	28.5	1.46 (3H, <i>s</i>)	28.3
16	4.12 (2H, <i>d</i> , $J = 6.5$)	26.8	4.09 (2H, <i>d</i> , $J = 6.6$)	26.5
17	5.26 (1H, <i>t</i> , $J = 6.5$)	124.6	5.27 (1H, <i>t</i> , $J = 6.6$)	123.1
18	–	131.6	–	131.8
19	1.82 (3H, <i>s</i>)	18.3	1.83 (3H, <i>s</i>)	18.1
20	1.65 (3H, <i>s</i>)	25.9	1.70 (3H, <i>s</i>)	25.6
1-OH	13.93 (1H, <i>s</i>)	–	13.70 (1H, <i>s</i>)	–
6-OH	–	–	–	–
7-OCH ₃	3.80 (3H, <i>s</i>)	61.3	3.81 (3H, <i>s</i>)	61.8

Table S10. ¹H NMR (500 MHz, δ_{H} , multi, (J in Hz) and ¹³C NMR (125 MHz) data of compound **10** in acetone- d_6 .

No.	10 (acetone- d_6)		Fuscaxanthone A (acetone- d_6)	
	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)
1	–	158.9	–	157.9
2	–	104.7	–	104.5
3	–	160.7	–	159.8
4	6.26 (1H, <i>s</i>)	94.7	6.24 (1H, <i>s</i>)	94.1
4a	–	157.2	–	156.2
5	6.87 (1H, <i>s</i>)	102.9	6.83 (1H, <i>s</i>)	101.6
6	–	156.3	–	154.5
7	–	142.1	–	142.7
8	–	138.3	–	137.0
8a	–	112.0	–	112.2

No.	10 (acetone- d_6)		Fuscaxanthone A (acetone- d_6)	
	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)
9	–	182.5	–	181.9
9a	–	103.6	–	103.7
10	–	–	–	–
10a	–	157.8	–	155.7
11	6.68 (1H, d , $J = 10.0$)	116.0	6.72 (1H, d , $J = 10.0$)	115.7
12	5.72 (1H, d , $J = 10.0$)	128.5	5.56 (1H, d , $J = 10.0$)	127.1
13	–	78.3	–	77.9
14	1.46 (3H, s)	28.5	1.46 (3H, s)	28.3
15	1.46 (3H, s)	28.5	1.46 (3H, s)	28.3
16	4.13 (2H, d , $J = 6.5$)	26.8	4.09 (2H, d , $J = 6.5$)	26.5
17	5.28 (1H, m)	124.7	5.26 (1H, m)	123.2
18	–	135.3	–	135.6
19	1.98 (2H, m)	40.5	2.01 (2H, m)	39.7
20	2.05 (2H, m)	27.3	2.04 (2H, m)	26.4
21	5.04 (1H, m)	125.2	5.02 (1H, m)	124.2
22	–	131.6	–	131.2
23	1.52 (3H, s)	17.8	1.54 (3H, s)	17.6
24	1.84 (3H, s)	16.5	1.82 (3H, s)	16.5
25	1.56 (3H, s)	25.7	1.60 (3H, s)	25.6
1-OH	13.93 (1H, s)	–	13.55 (1H, s)	–
6-OH	9.71 (1H, s)	–	6.15 (1H, s)	–
7-OCH ₃	3.80 (3H, s)	61.4	3.73 (3H, s)	62.0

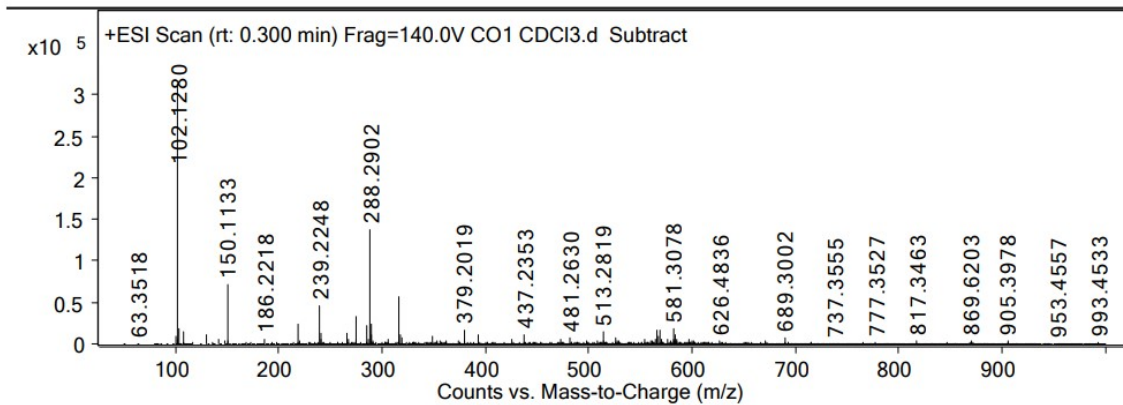
Table S11. ¹H NMR (500 MHz, δ_{H} , multi, (J in Hz) and ¹³C NMR (125 MHz) spectral data comparison of compound **11** in acetone- d_6 .

No.	11 (acetone- d_6)		11-hydroxy-1-isomangostin (acetone- d_6)	
	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)	δ_{H} (ppm) J (Hz)	δ_{C} (ppm)
1	–	156.0	–	155.9
2	–	105.5	–	105.0
3	–	161.2	–	161.0
4	6.39 (1H, s)	94.1	6.40 (1H, s)	94.2
4a	–	157.6	–	157.6
4b	–	154.9	–	154.9
5	6.71 (1H, s)	102.1	6.72 (1H, s)	102.1
6	–	155.6	–	155.8

No.	11 (acetone- <i>d</i> ₆)		11-hydroxy-1-isomangostin (acetone- <i>d</i> ₆)	
	δ_{H} (ppm) <i>J</i> (Hz)	δ_{C} (ppm)	δ_{H} (ppm) <i>J</i> (Hz)	δ_{C} (ppm)
7	–	144.4	–	144.3
8	–	137.7	–	137.6
8a	–	115.4	–	115.1
9	–	176.1	–	176.3
9a	–	107.9	–	107.7
10	2.57 (1H, <i>dd</i> , <i>J</i> = 16.8, 7.8) 2.92 (1H, <i>dd</i> , <i>J</i> = 16.8, 5.8)	27.1	2.56 (1H, <i>dd</i> , <i>J</i> = 16.8, 7.8) 2.94 (1H, <i>dd</i> , <i>J</i> = 16.8, 5.7)	27.1
11	3.81 (1H, <i>dd</i> , <i>J</i> = 8, 5.5)	69.1	3.82 (1H, <i>dd</i> , <i>J</i> = 7.8, 5.7)	69.0
12	–	78.6	–	78.5
13	1.30 (3H, <i>s</i>)	20.6	1.30 (3H, <i>s</i>)	20.6
14	1.43 (3H, <i>s</i>)	26.0	1.43 (3H, <i>s</i>)	26.0
15	4.09 (2H, <i>t</i> , <i>J</i> = 6)	26.6	4.09 (2H, <i>d</i> , <i>J</i> = 6.8)	26.6
16	5.31 (1H, <i>t</i> , <i>J</i> = 6.8)	125.6	5.31 (1H, <i>br t</i> , <i>J</i> = 6.8)	125.8
17	–	130.2	–	130.5
18	1.82 (3H, <i>s</i>)	26.1	1.81 (3H, <i>br s</i>)	26.1
19	1.65 (3H, <i>s</i>)	18.3	1.64 (3H, <i>br s</i>)	18.3
7-OMe	3.77 (3H, <i>s</i>)	61.2	3.77 (3H, <i>s</i>)	61.0

Table S12. Alpha-glucosidase inhibition (IC₅₀) by extracts of studied plant

Bio-source		IC ₅₀
Extract	Crude MeOH	27.7 ± 0.5 µg/mL
	Extract H	>200 µg/mL
	Extract EA	66.0 ± 2.6 µg/mL
Fraction	Fractions EA1-EA5	>200 µg/mL
	Fraction EA6	12.0 ± 0.4 µg/mL
	Fractions EA7-EA11	>200 µg/mL
	Fraction EA12	60.9 ± 1.2 µg/mL
	Fraction EA13	>200 µg/mL
	Fraction EA14	>200 µg/mL
	Fraction EA15	66.9 ± 3.7 µg/mL
	Fraction EA16	155.9 ± 4.4 µg/mL



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535.34	505.45
535.4021	464
535.4724	285.27
536.2408	315.57
536.3544	482.45
536.355	367.71
537.2214	389.98
537.2855	258.96
537.3175	1644.98
537.4089	211.38
538.222	408.70
538.3198	753.27
538.3705	551.23
538.4315	2609.87
538.61	324.96
538.9174	213.55
539.1318	204.8
539.2621	864.14
539.2941	1170.32
539.3386	724.5
539.3704	451.58
539.4331	662.92
540.2837	838.01
540.334	1028.29
540.4314	805.96
540.5389	589.08
540.5925	249.86
541.1746	310.72
541.2671	1580.1
541.3711	1031.17
541.443	374.14
542.2172	231.78
542.252	796.59
542.3474	494.92
542.3848	428.57
543.1245	324.05
543.3859	1136.04
543.4429	218.1
543.5453	244.90
544.2002	207.88
544.2698	375.34
544.3806	614.06
544.4136	506.6
545.2855	875
545.2467	270.47
545.4182	270.35

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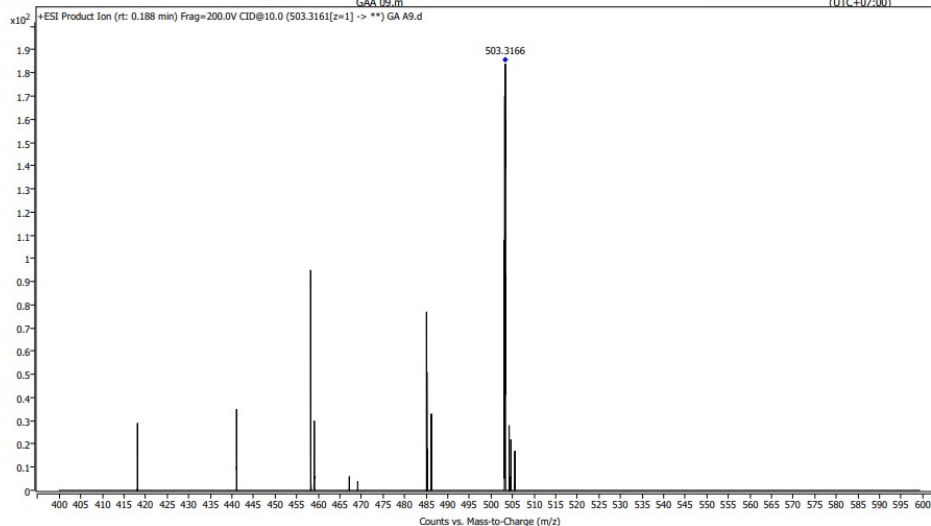
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User Spectrum Plot Report

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 Inj. Vol. (ul): 3 Plate Pos.: IRM Status: All ions missed
 Data File: GA A9.d Method (Acq): CO TUYEN 16112023 Comment: Acq. Time (Local): 17/11/2023 6:37:36 PM
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Figure S1A. The HRESIMS spectrum of 1.

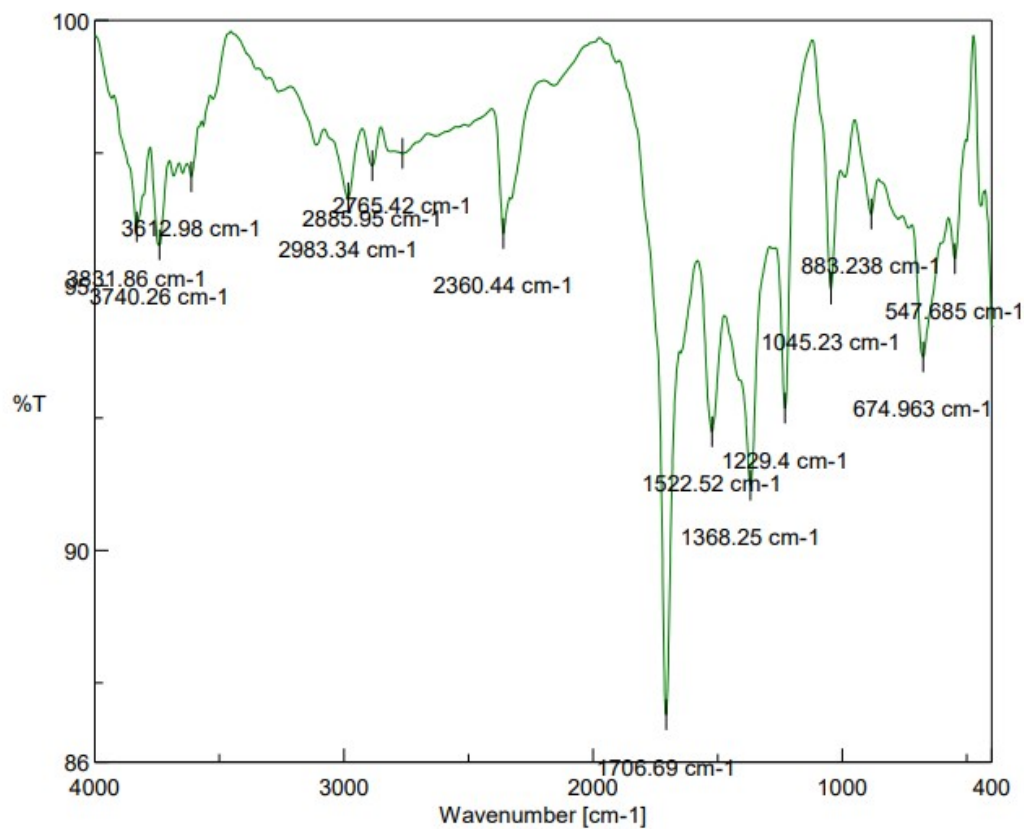
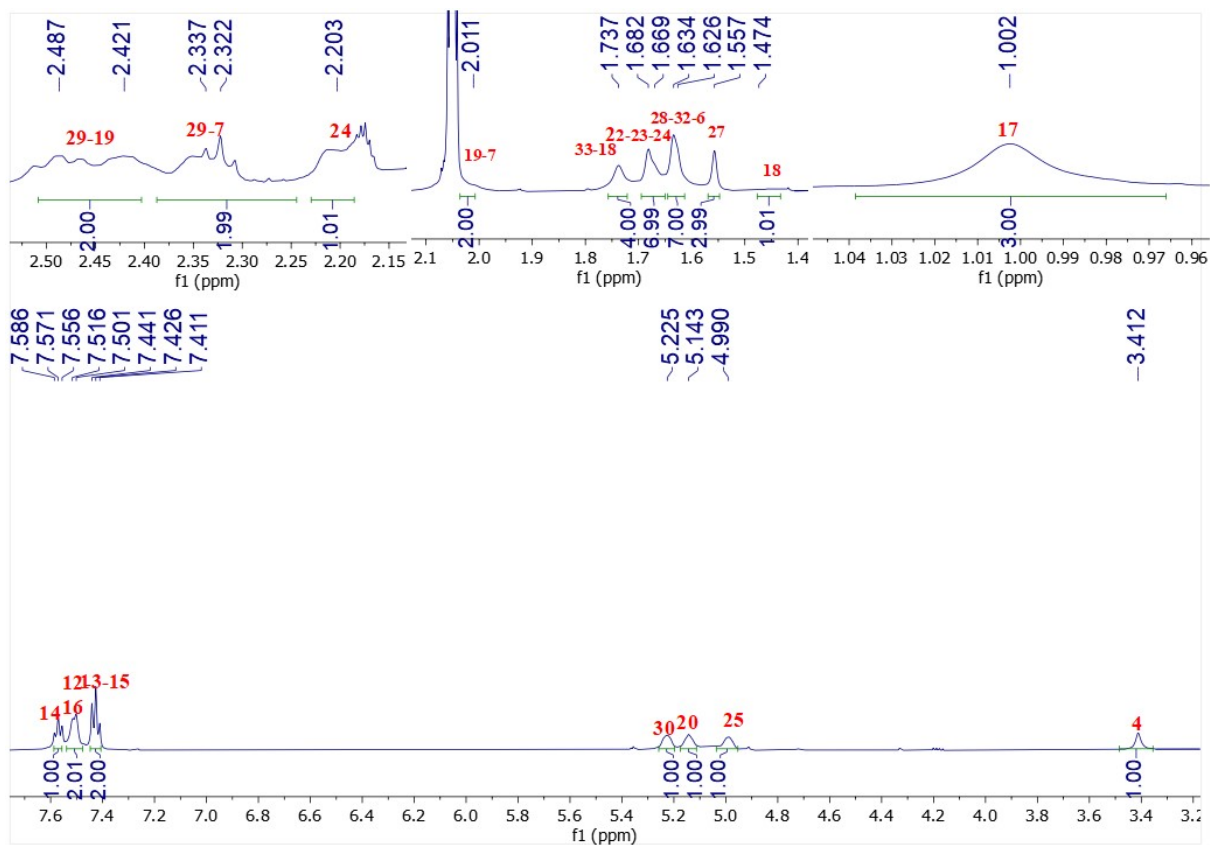


Figure S1B. The IR spectrum of 1.



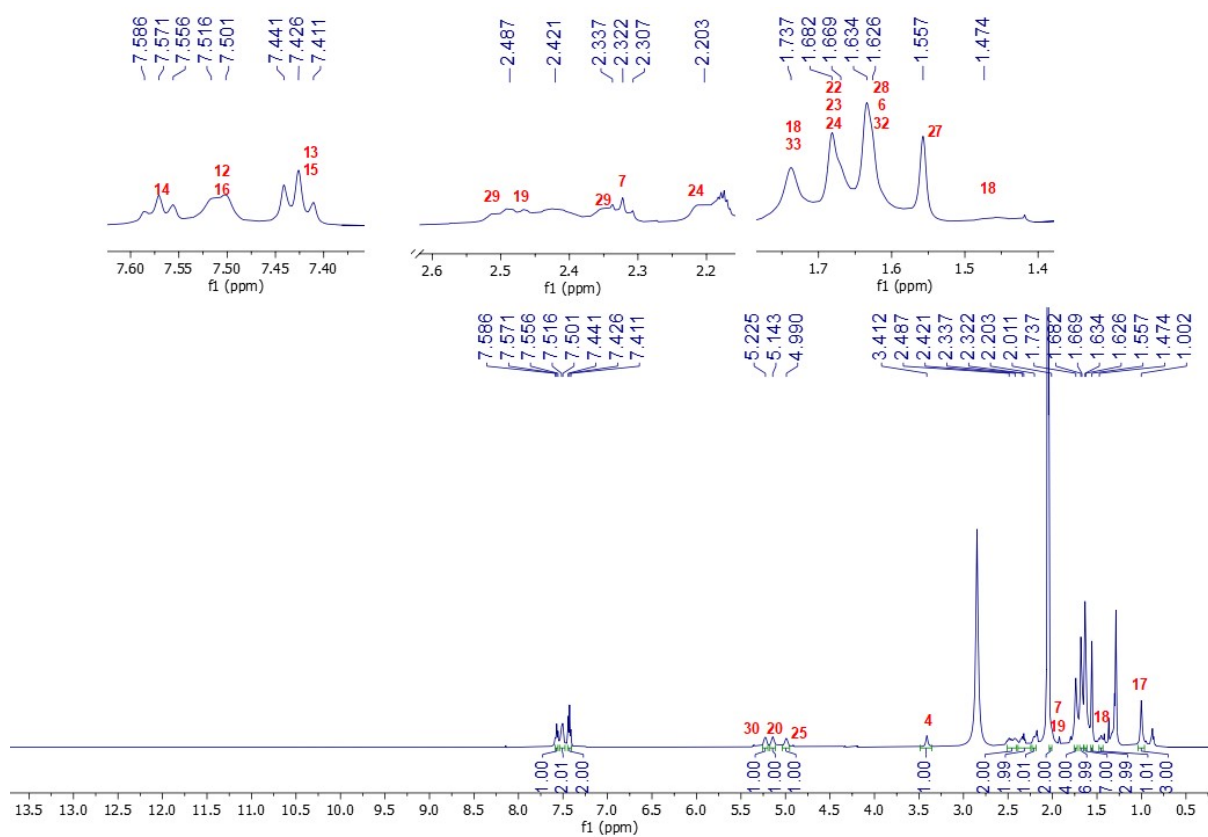
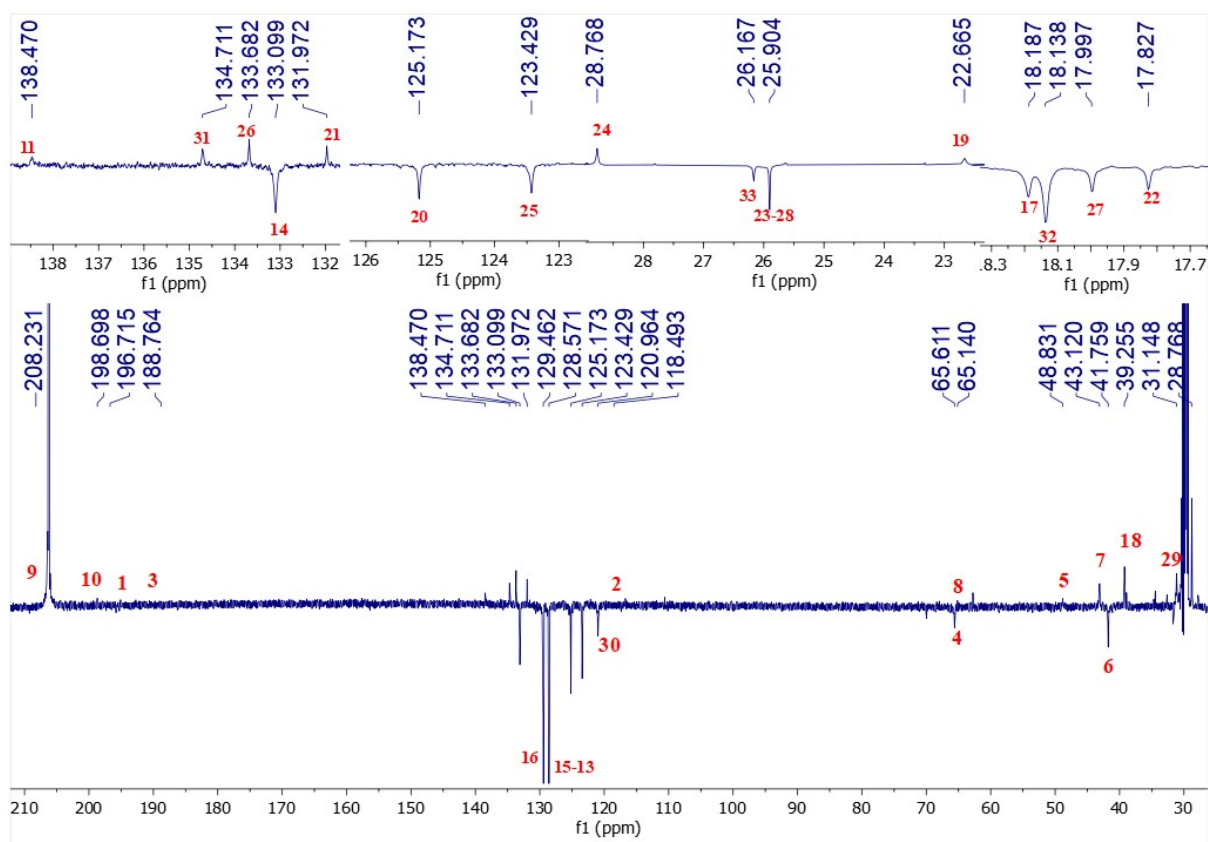


Figure S1C. The ^1H NMR spectrum of **1** in acetone- d_6 .



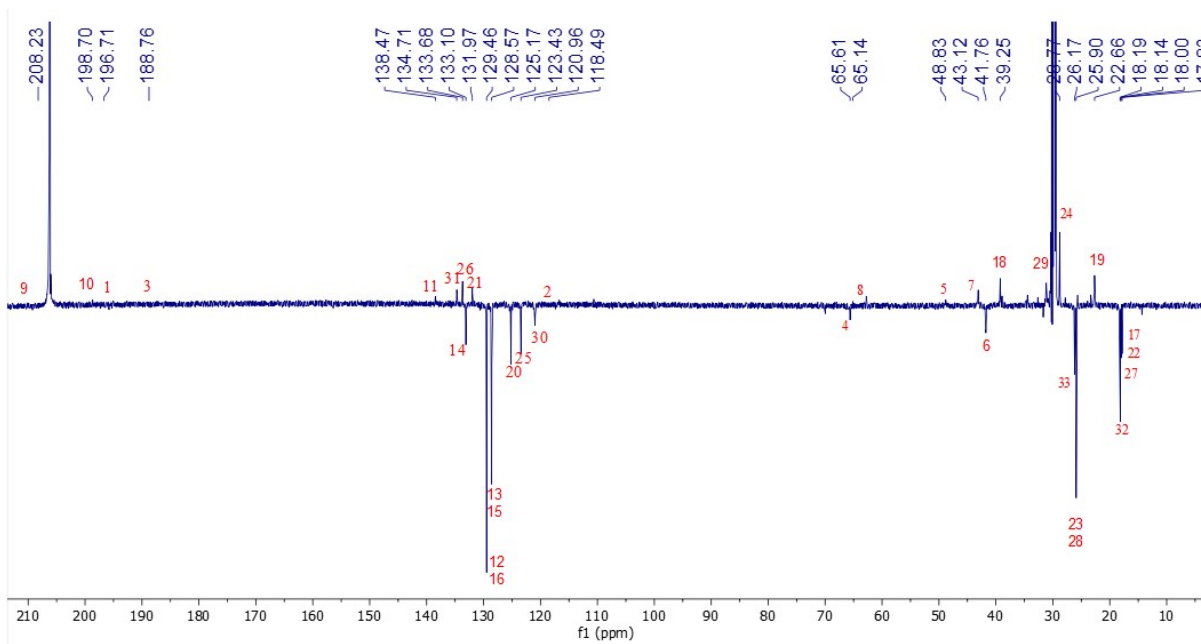


Figure S1D. The ^{13}C NMR spectrum of **1** in acetone- d_6 .

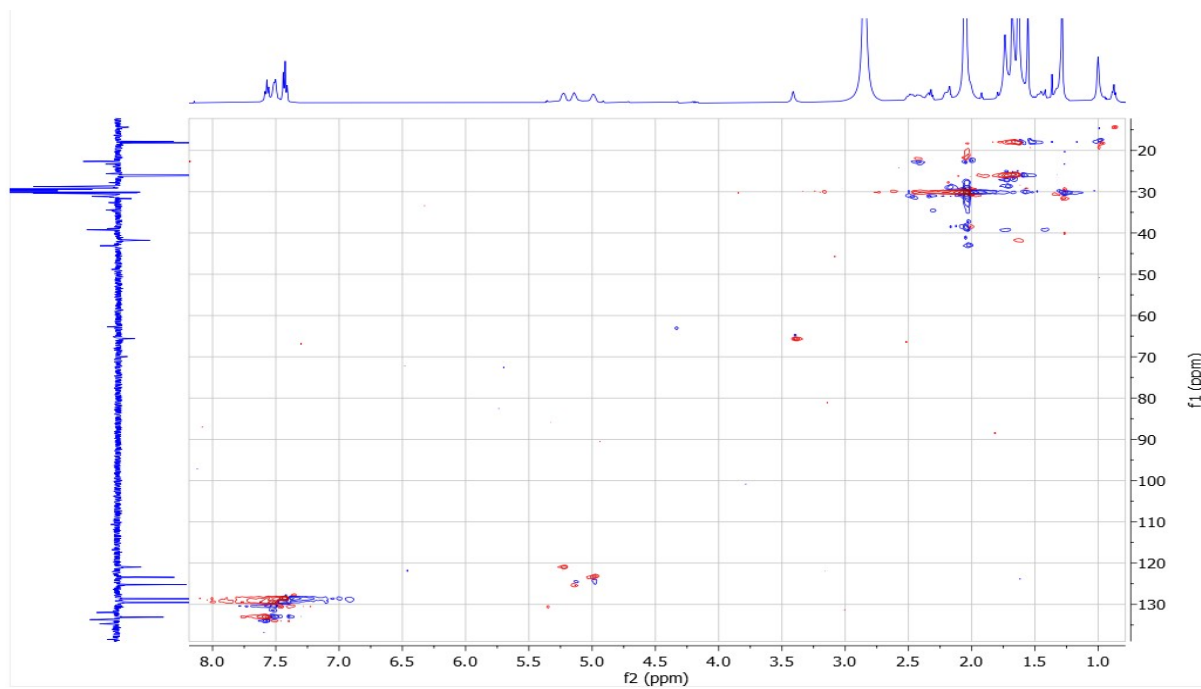


Figure S1E. The HSQC spectrum of **1** in acetone- d_6 .

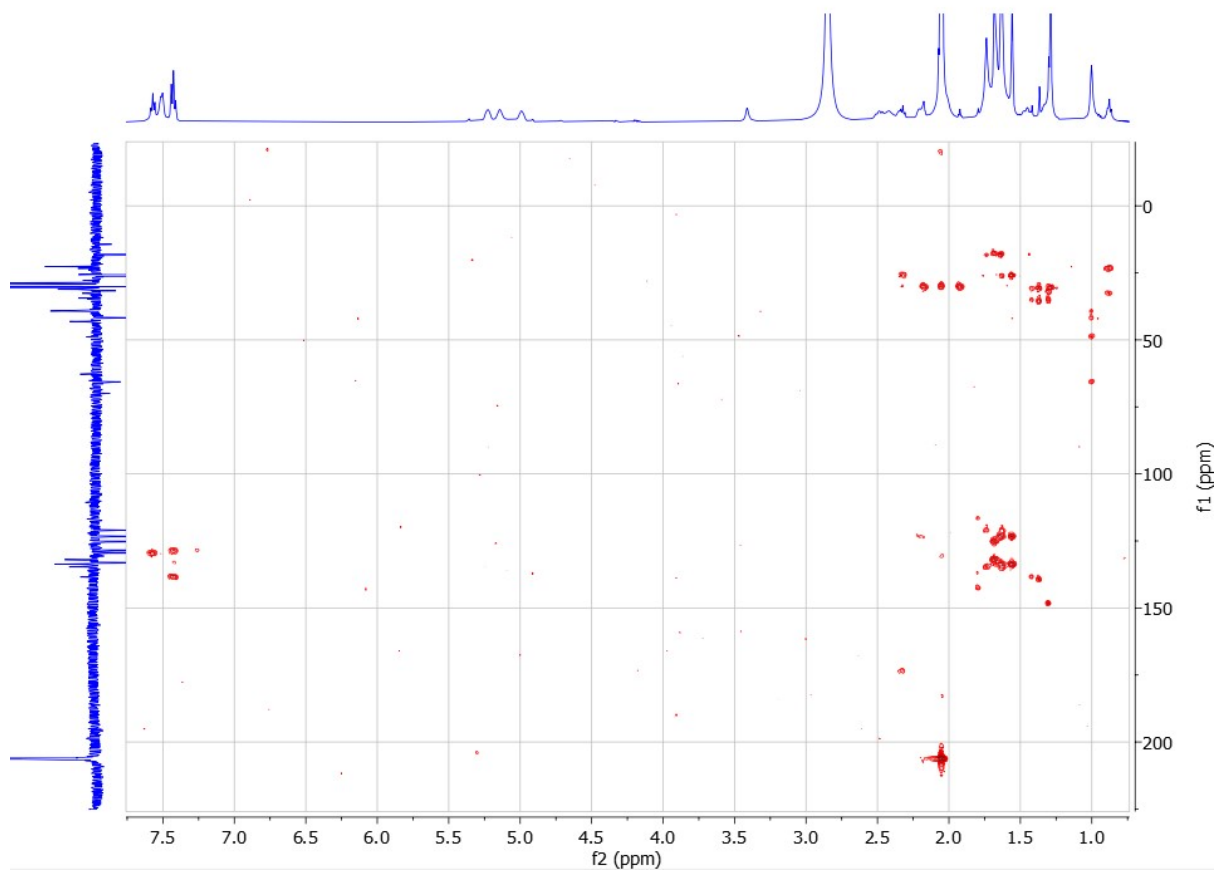


Figure S1F. The HMBC spectrum of **1** in acetone- d_6 .

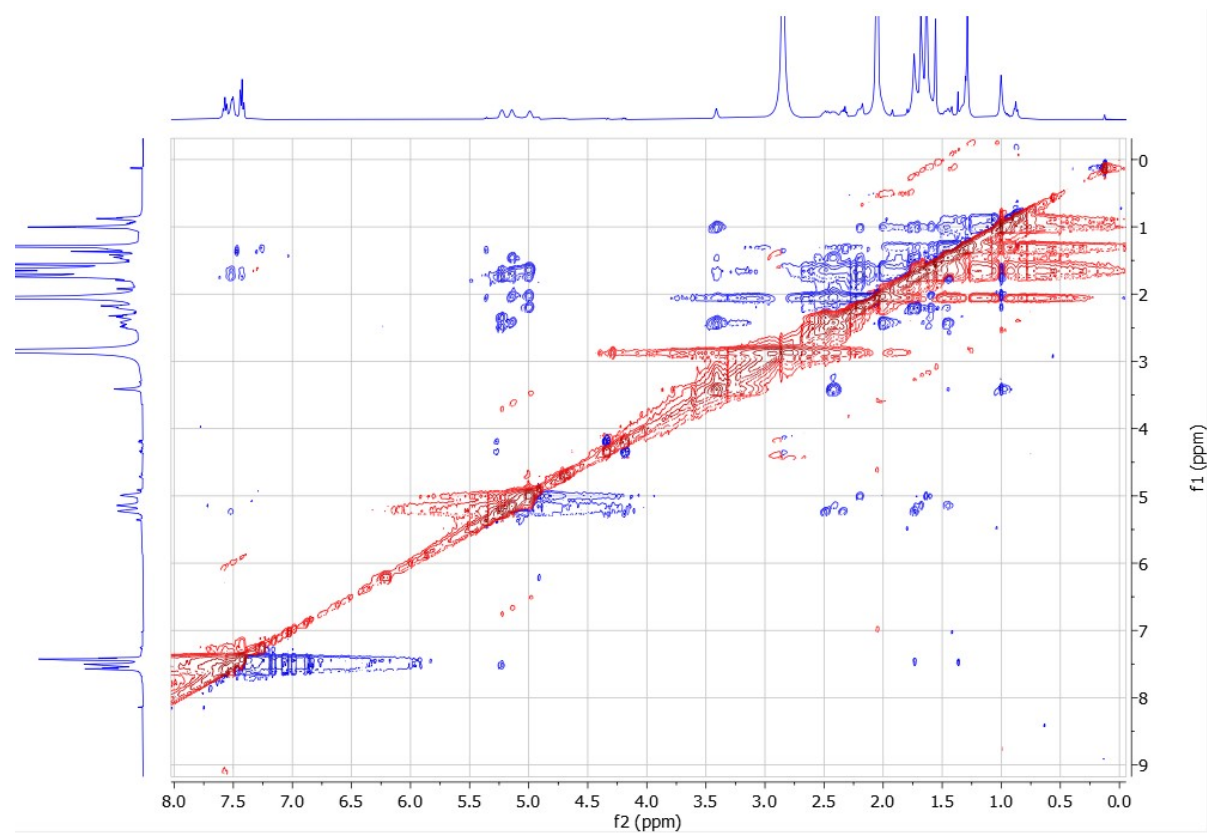


Figure S1G. The NOESY spectrum of **1** in acetone- d_6 .

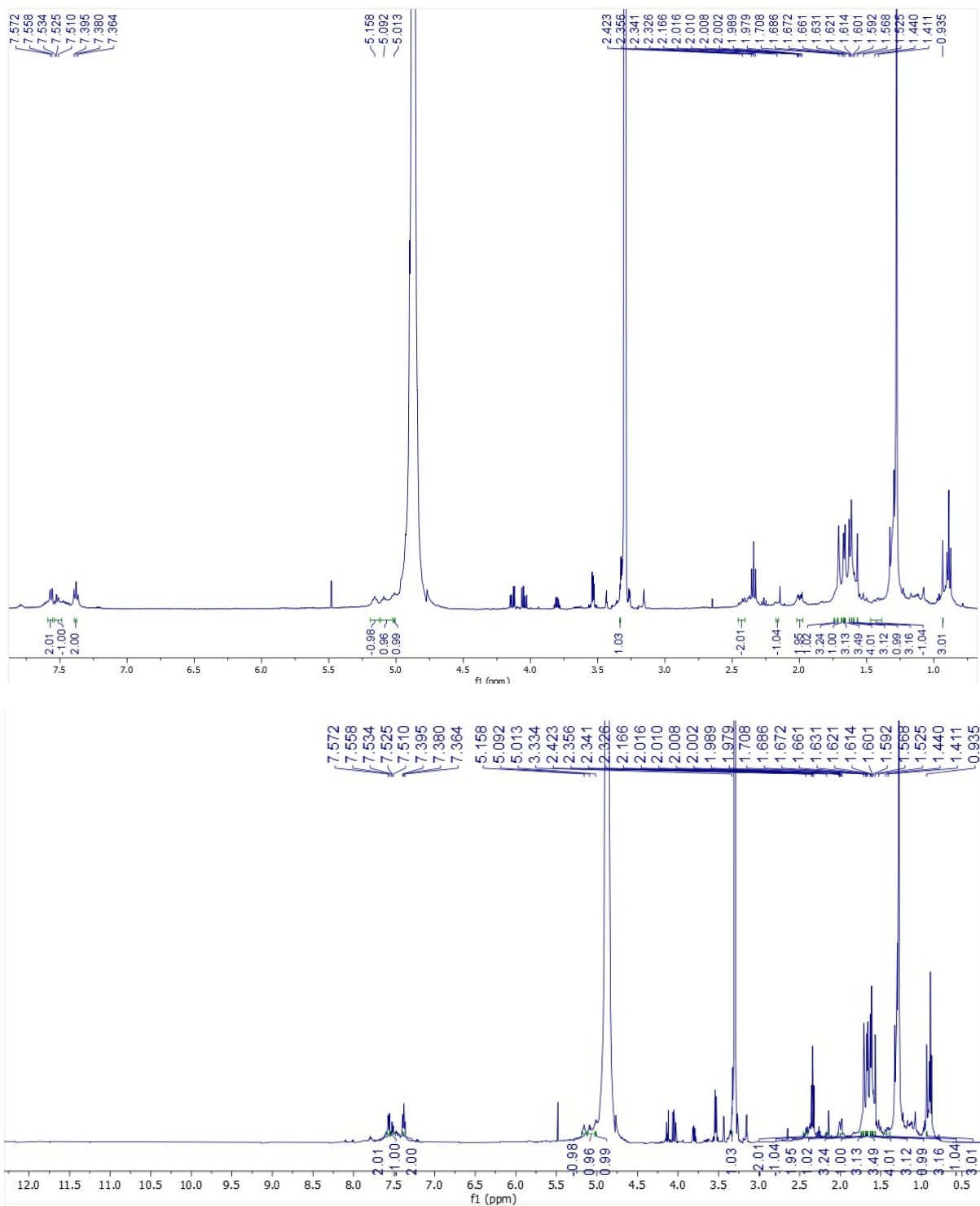


Figure S1H. The ^1H NMR spectrum of **1** in methanol- d_4 .

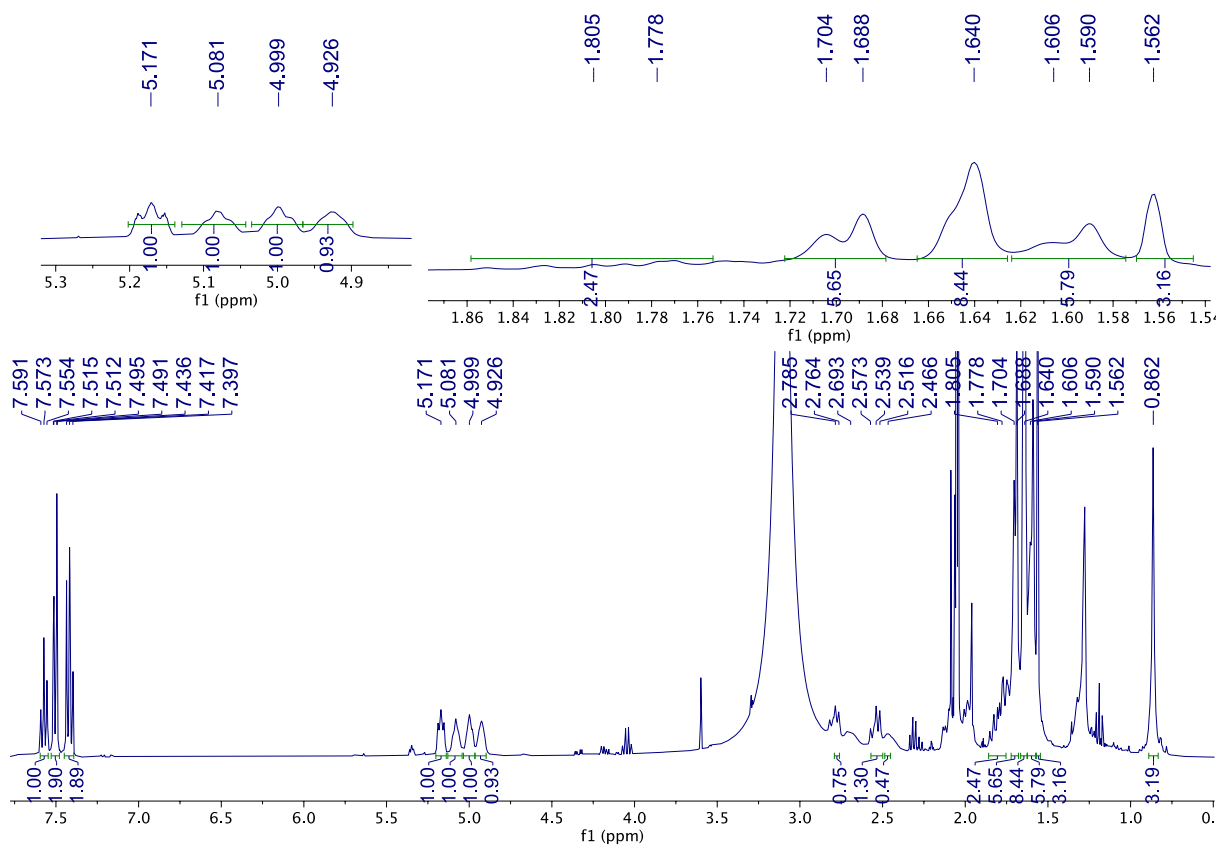


Figure S2A. The ^1H NMR spectrum of **2** in acetone- d_6 .

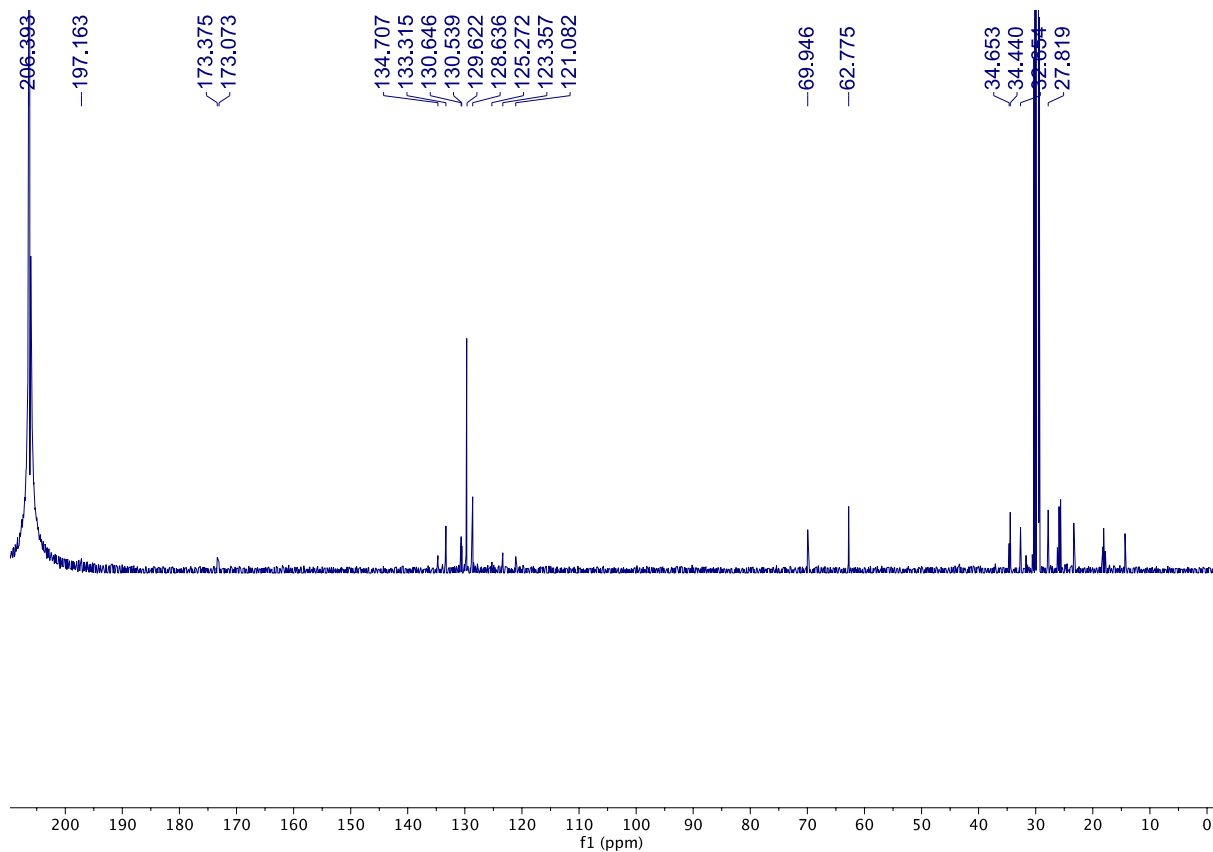


Figure S2B. The ^{13}C NMR spectrum of **2** in acetone- d_6 .

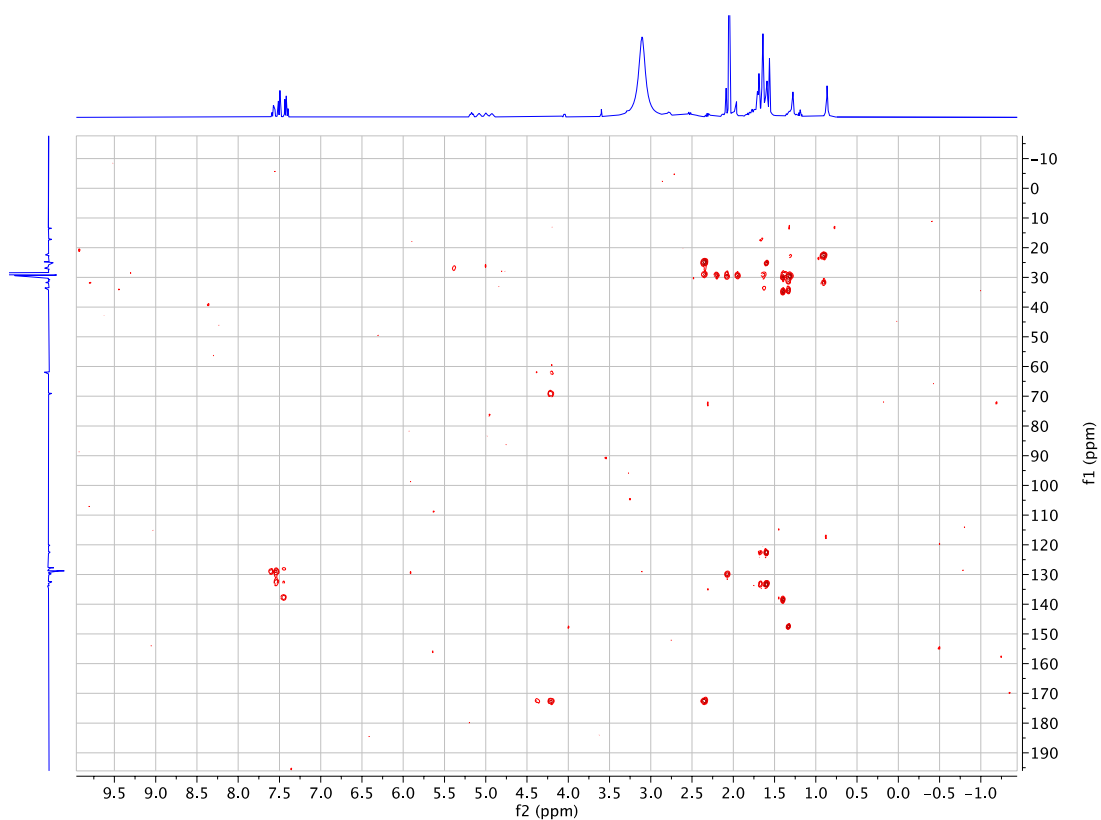


Figure S2C. The HMBC spectrum of **2** in acetone- d_6 .

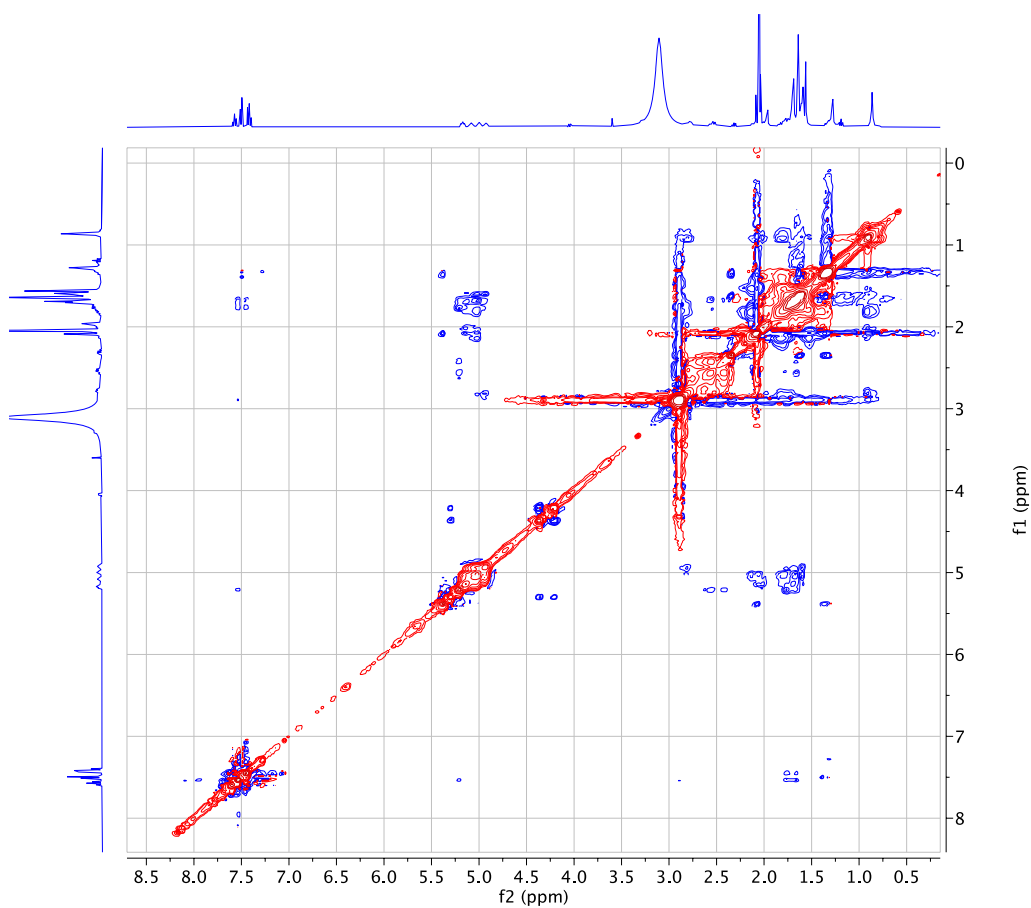


Figure S2D. The NOESY spectrum of **2** in acetone-*d*₆.

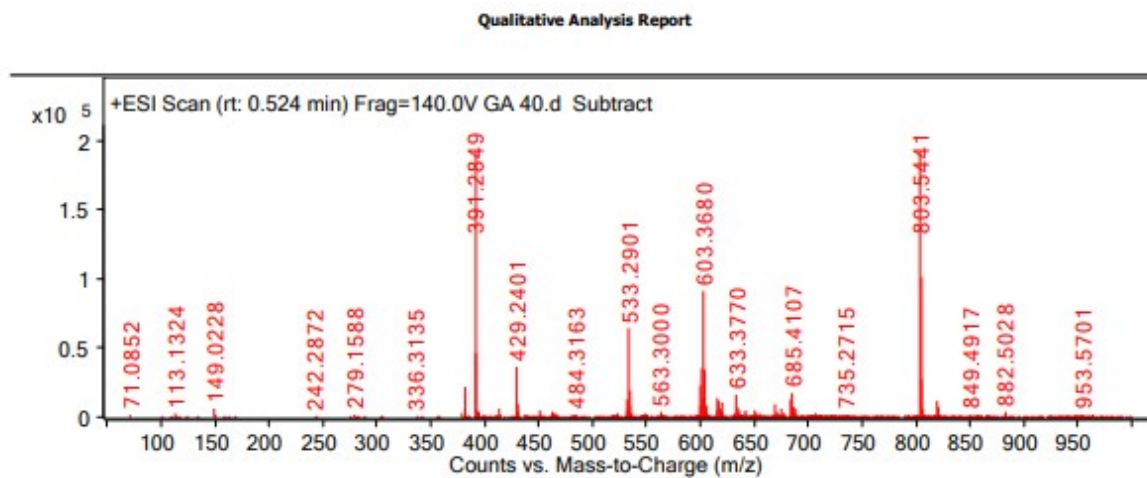
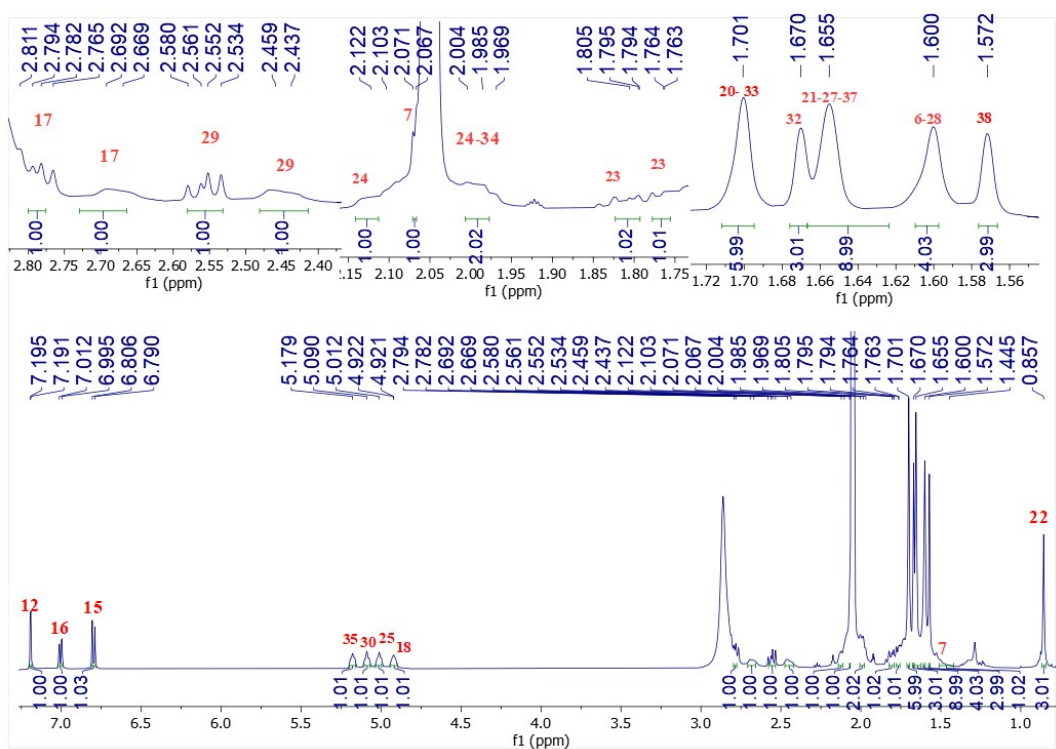


Figure S3A. The HRESIMS spectrum of **3**.



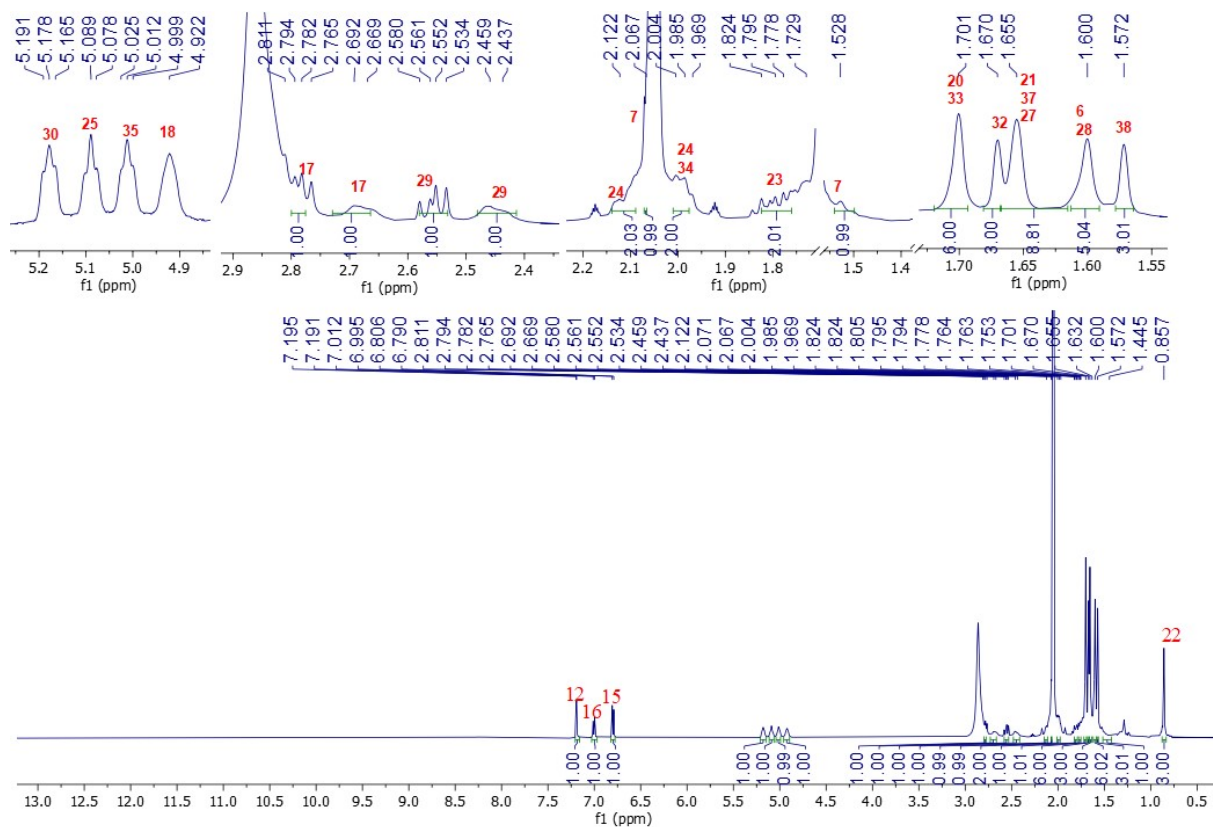


Figure S3B. The ^1H NMR spectrum of **3** in acetone- d_6 .

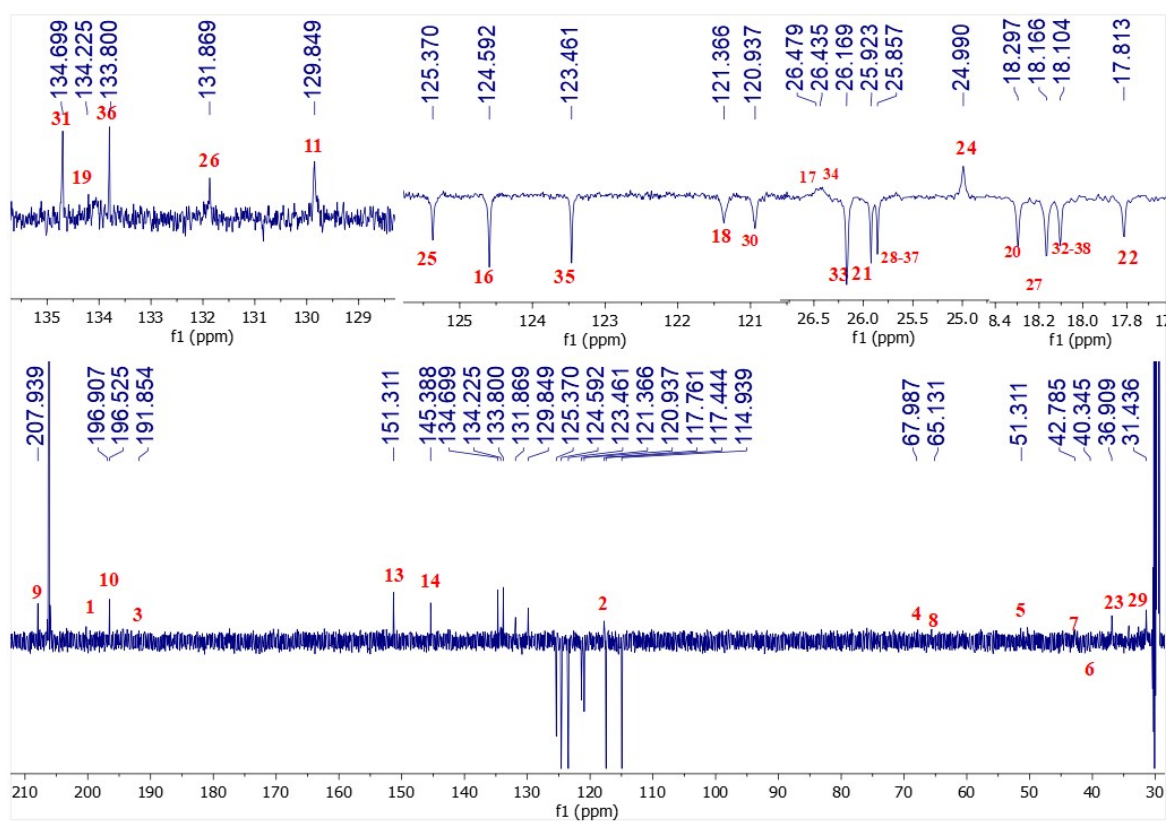


Figure S3C. The ^{13}C NMR spectrum of **3** in acetone- d_6 .

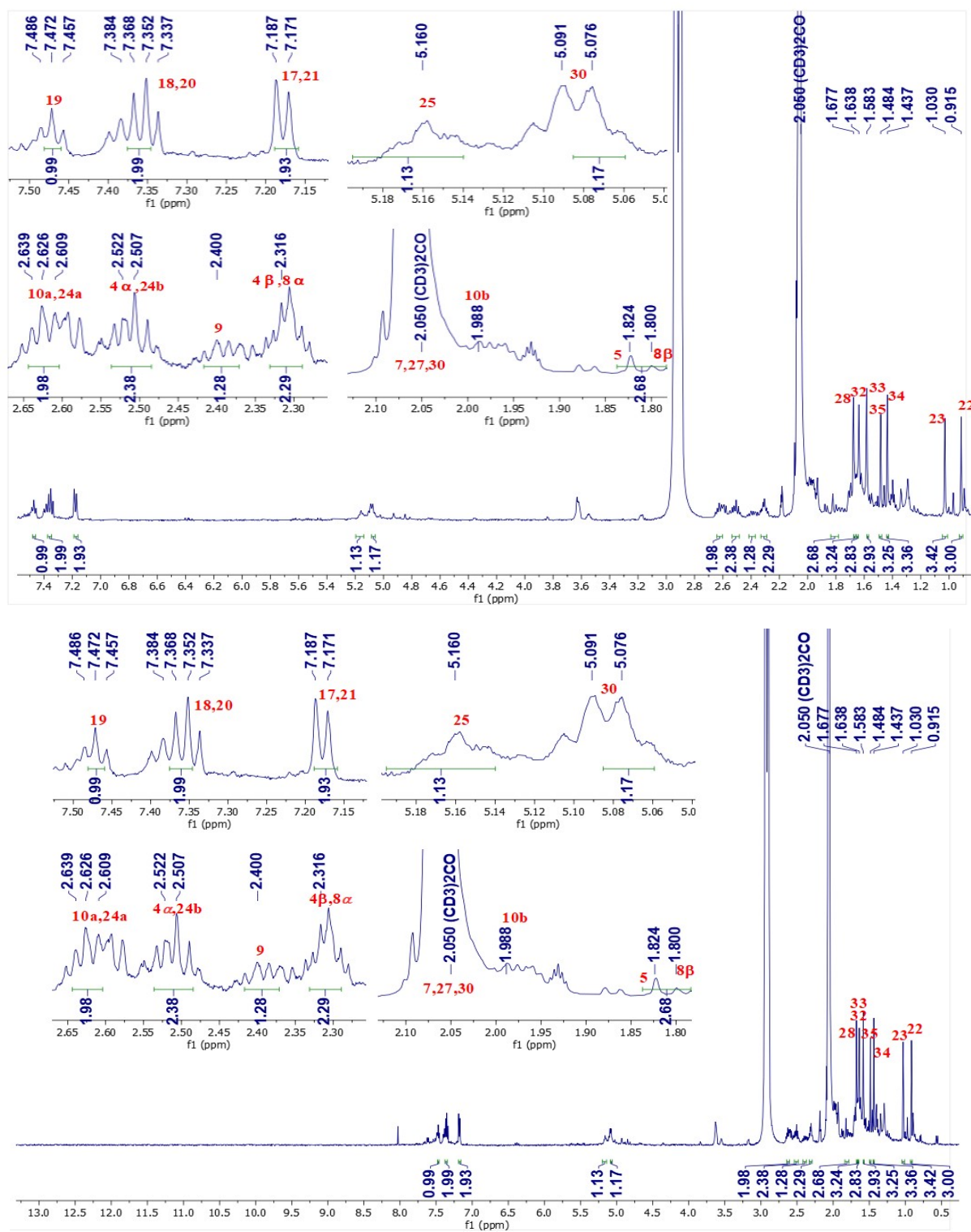


Figure S4A. The ^1H NMR spectrum of **4** in acetone- d_6 .

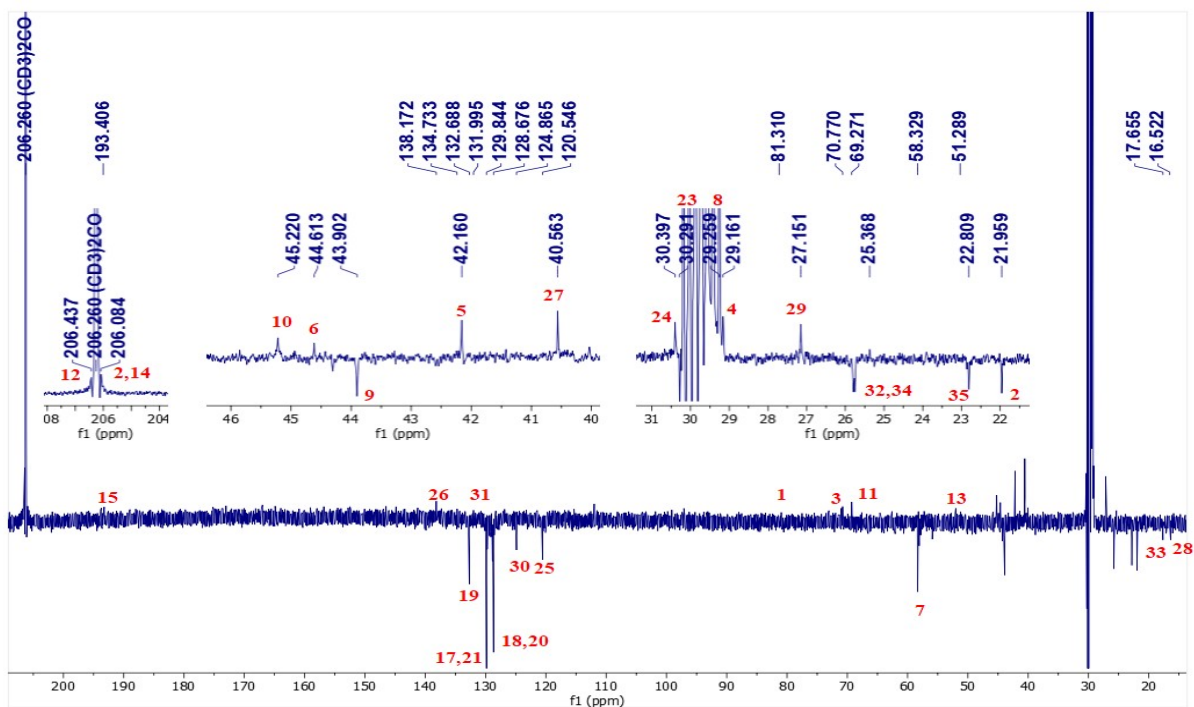


Figure S4B. The ^{13}C NMR spectrum of **4** in acetone- d_6 .

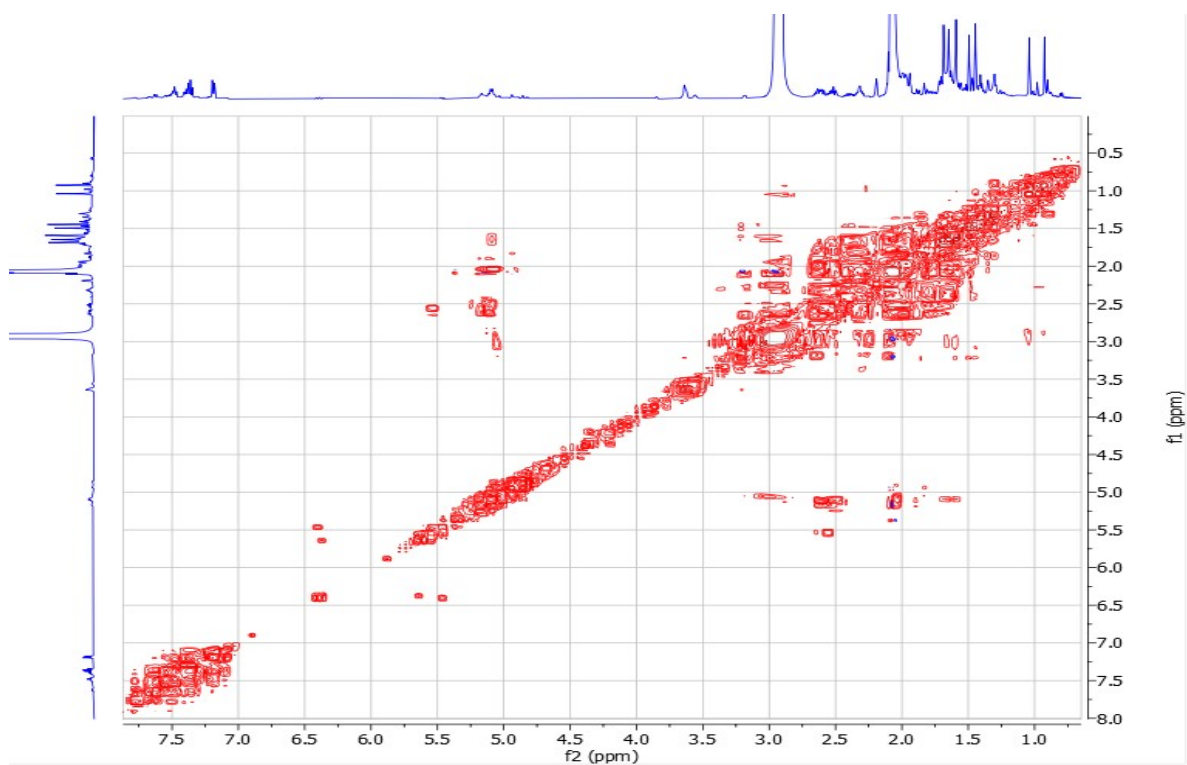


Figure S4C. The COSY spectrum of **4** in acetone- d_6 .

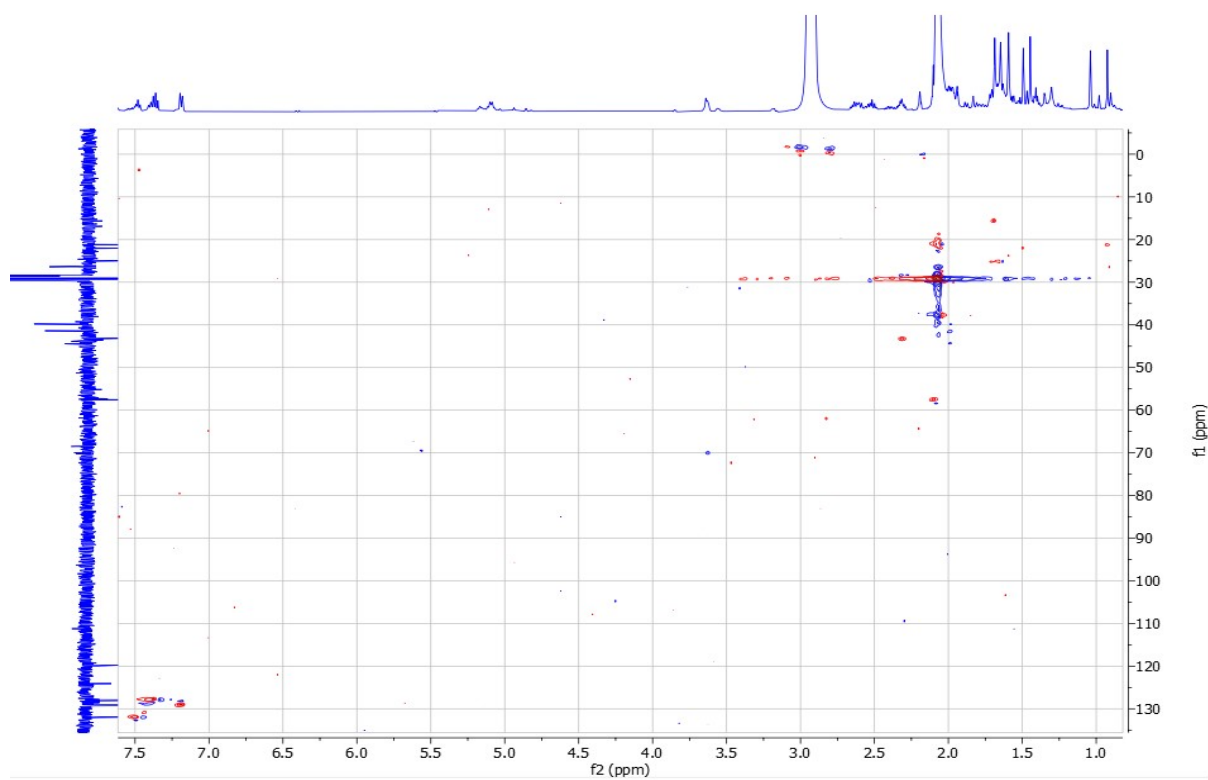


Figure S4D. The HSQC spectrum of **4** in acetone- d_6 .

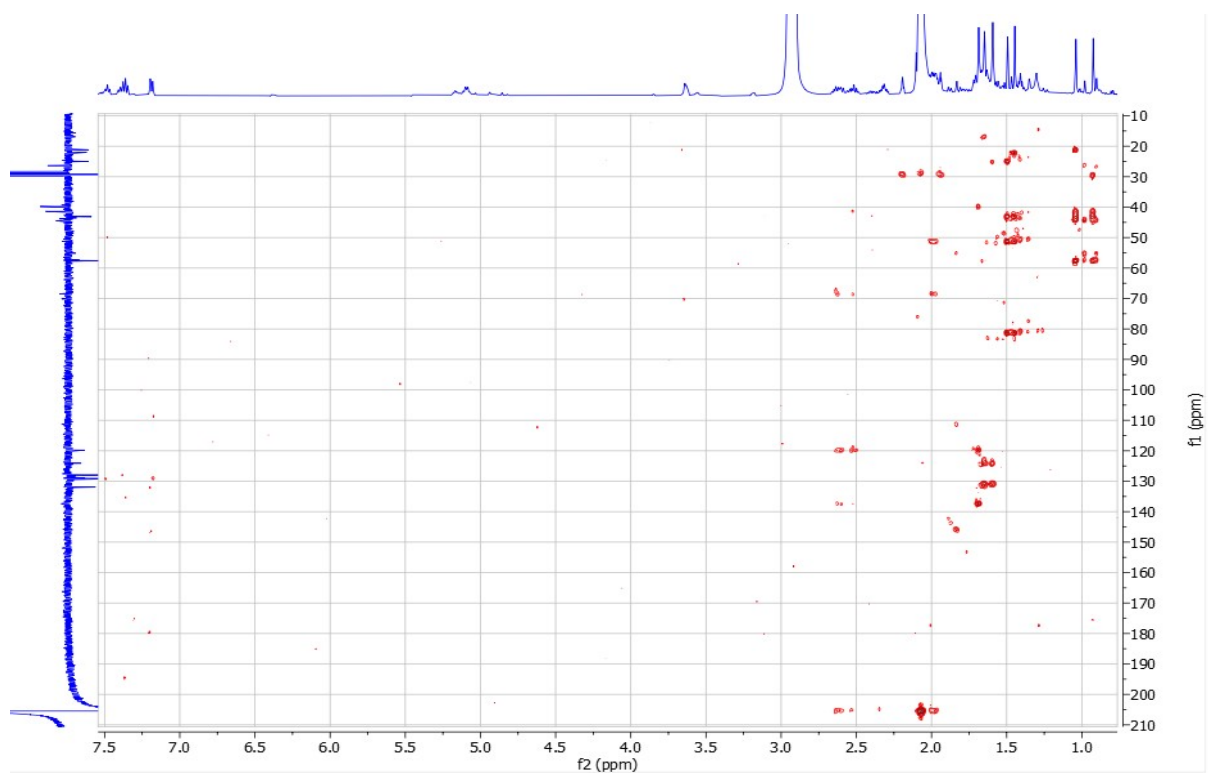


Figure S4E. The HMBC spectrum of **4** in acetone- d_6 .

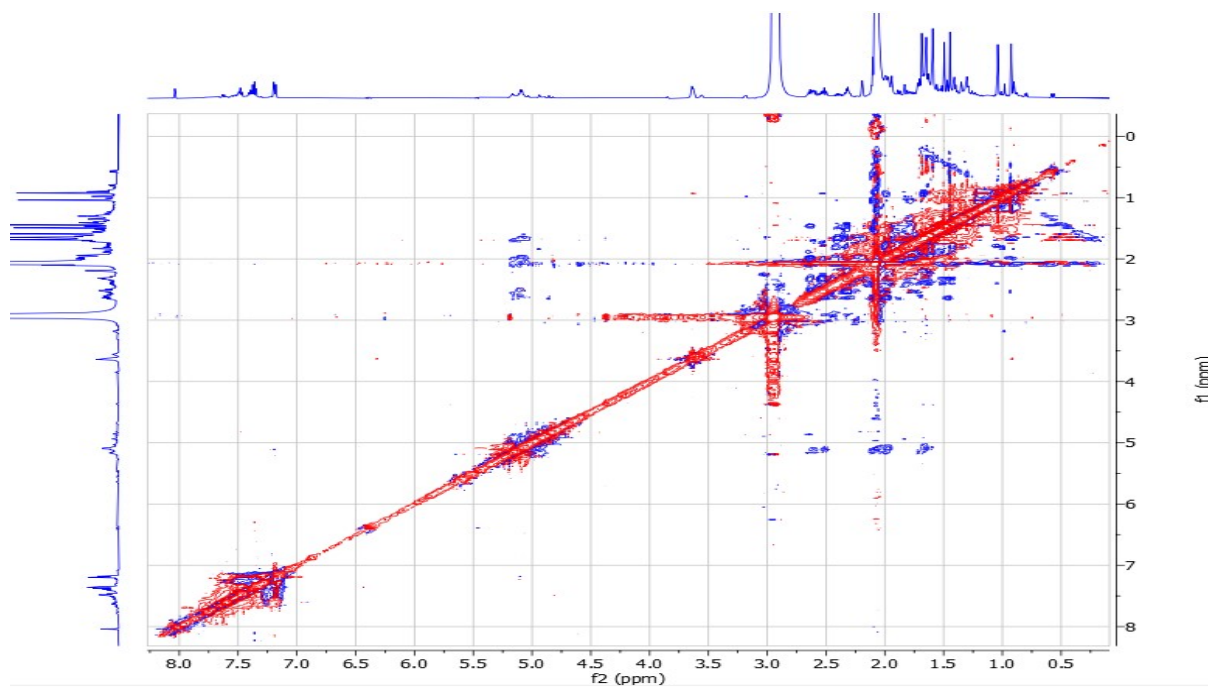


Figure S4F. The NOESY spectrum of **4** in acetone- d_6 .

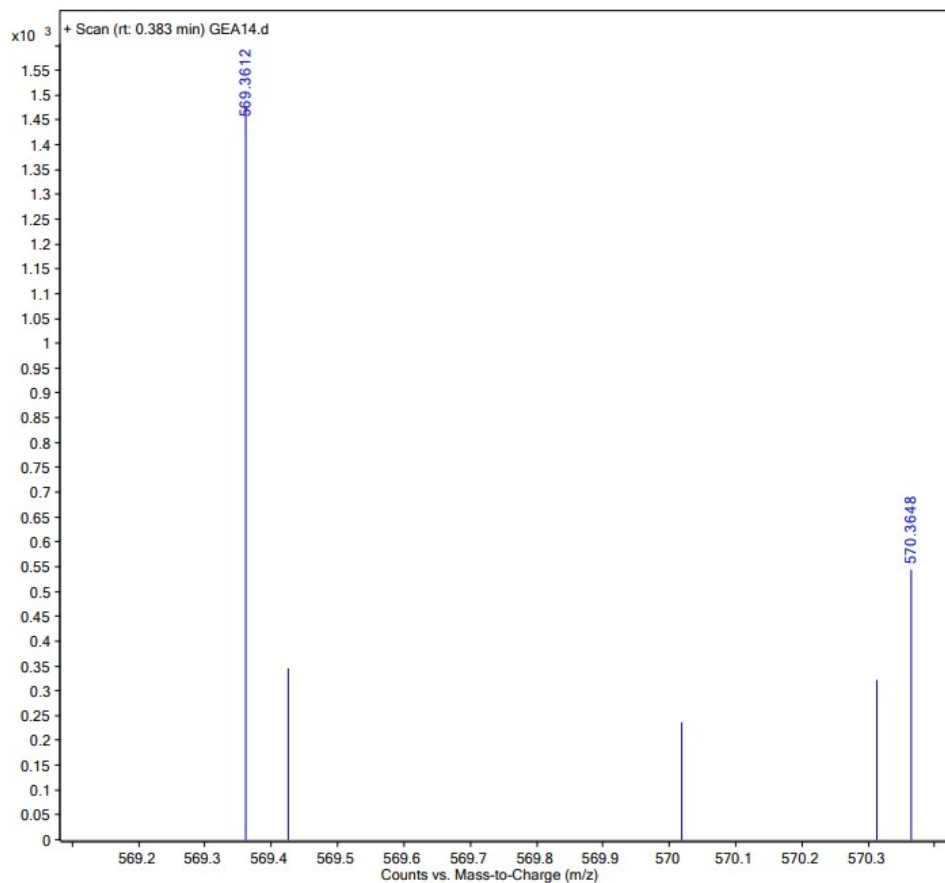
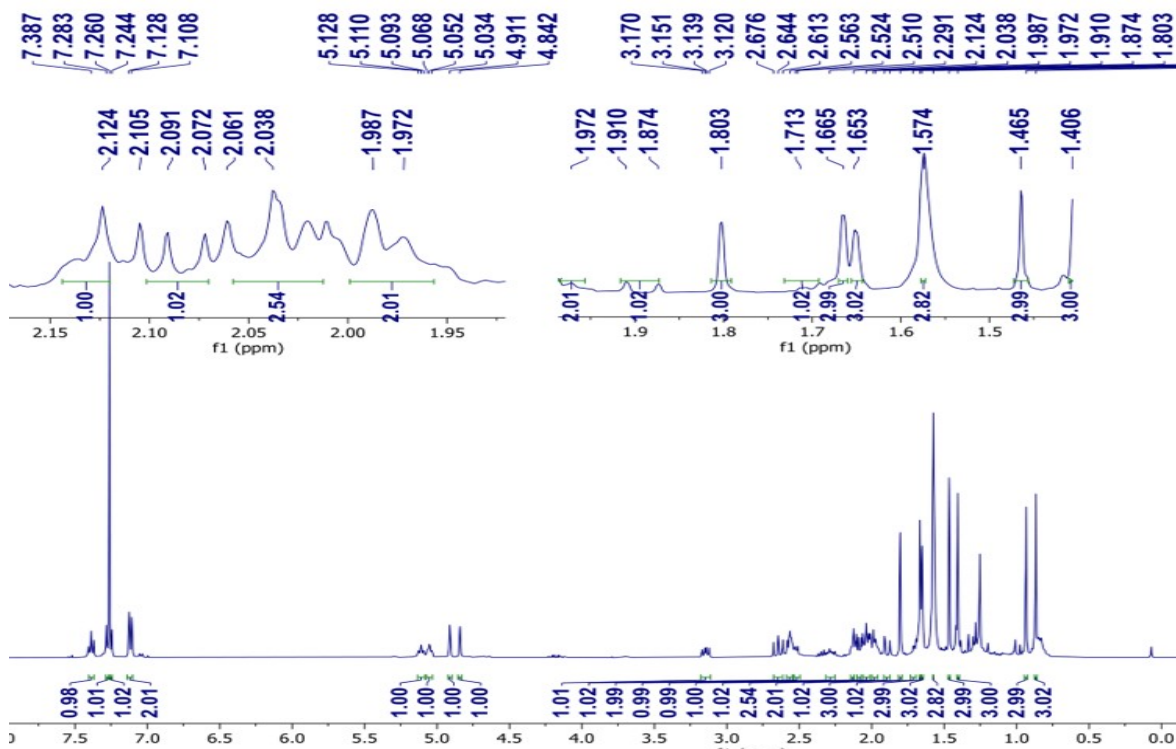


Figure S5A. The HRESIMS spectrum of **5**.



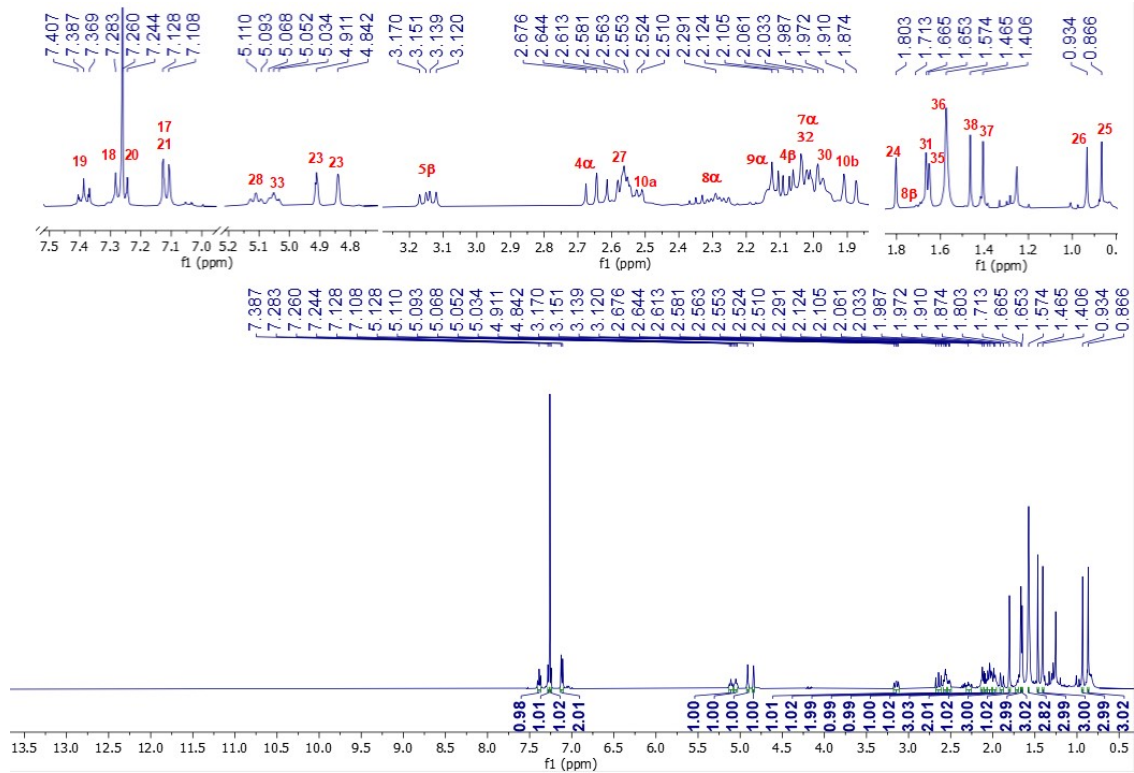


Figure S5B. The ^1H NMR spectrum of **5** in CDCl_3 .

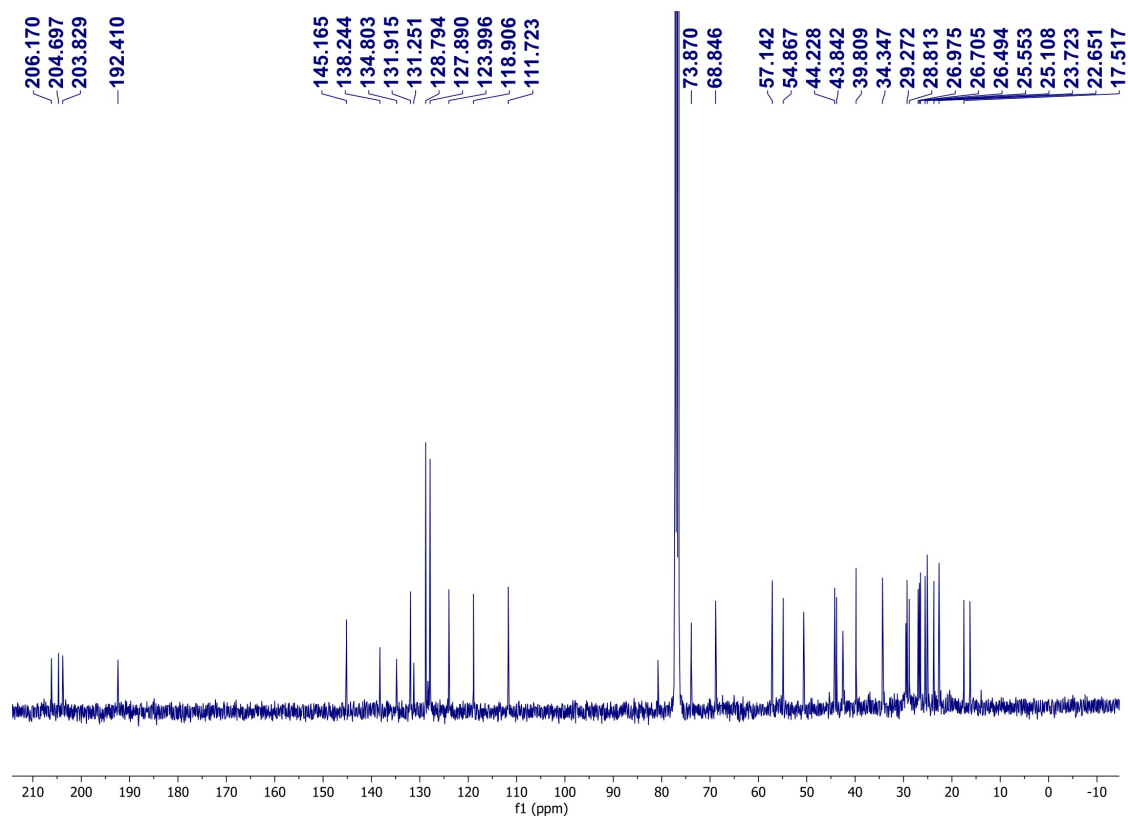


Figure S5C. The ^{13}C NMR spectrum of **5** in CDCl_3 .

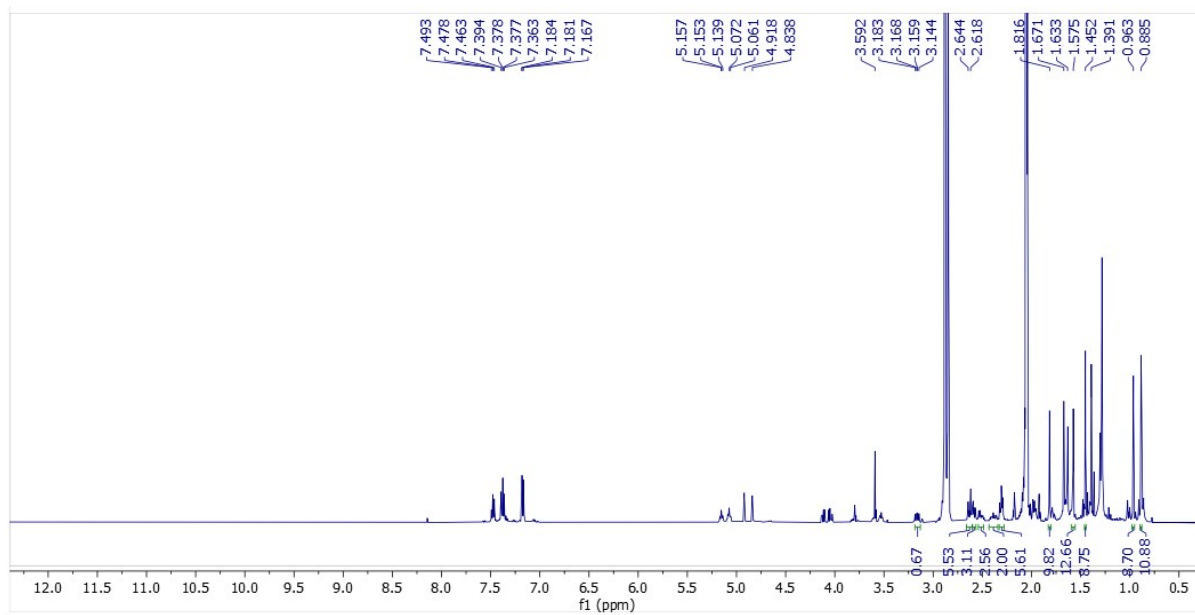
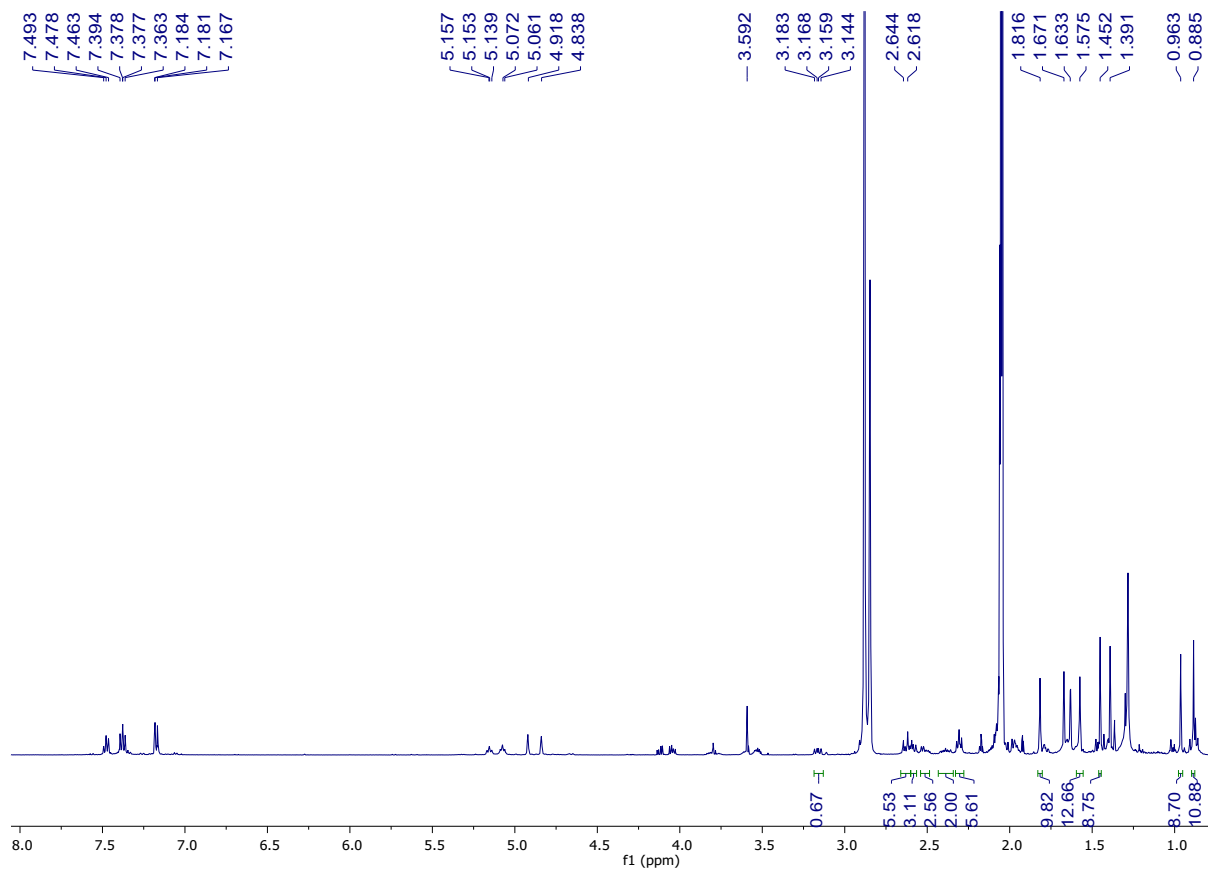


Figure S5D. The ^1H NMR spectrum of **5** in acetone- d_6 .

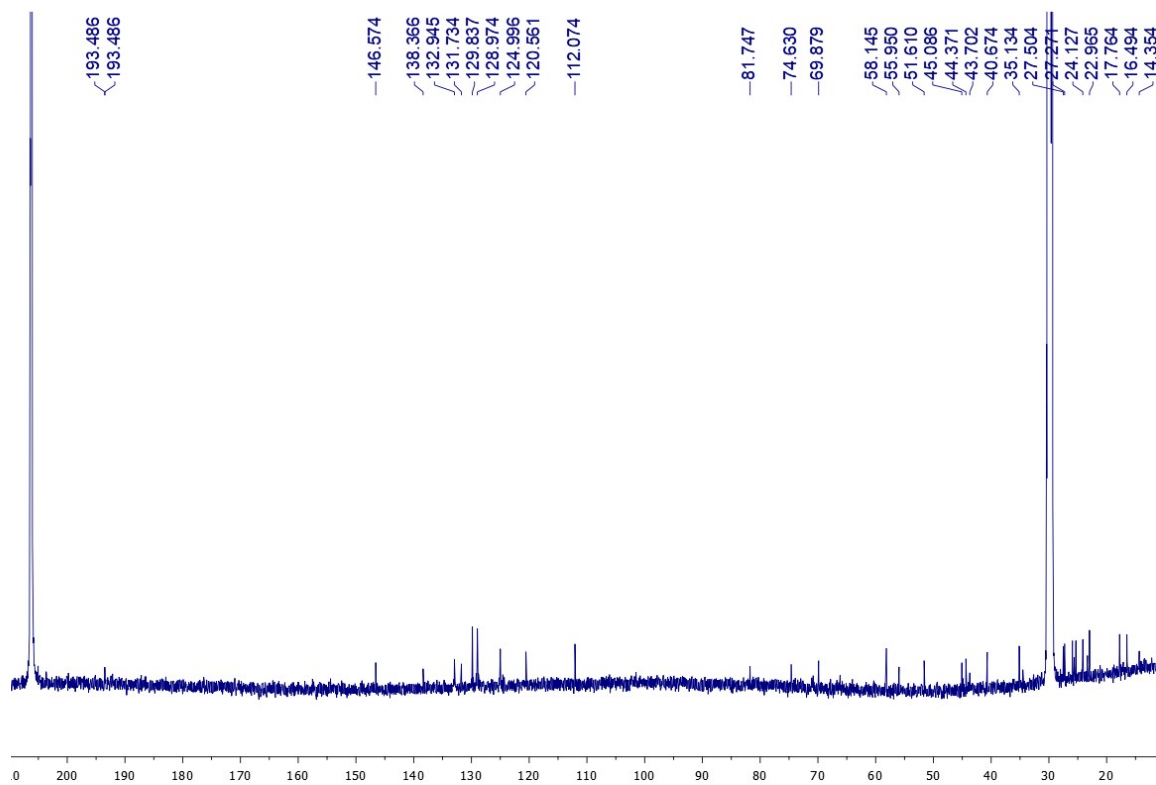


Figure S5E. The ^{13}C NMR spectrum of **5** in acetone- d_6 .

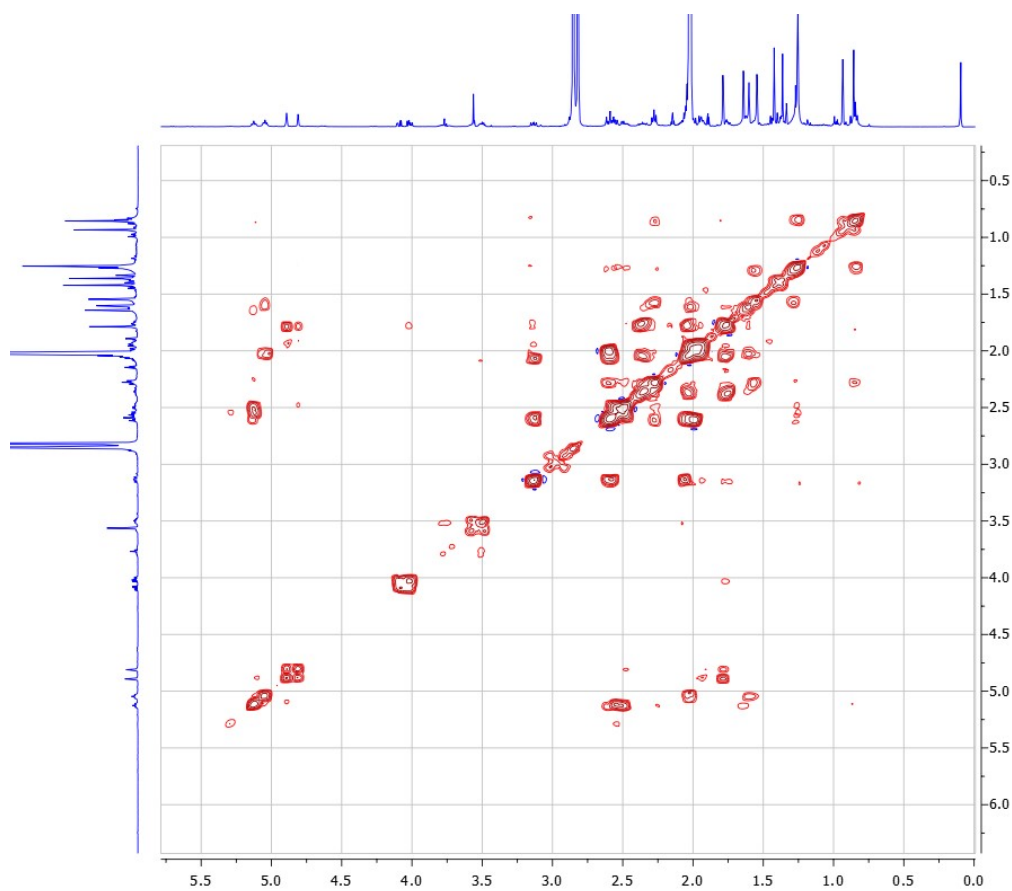


Figure S5F. The COSY spectrum of **5** in acetone- d_6 .



Figure S5G. The HSQC spectrum of **5** in acetone- d_6 .

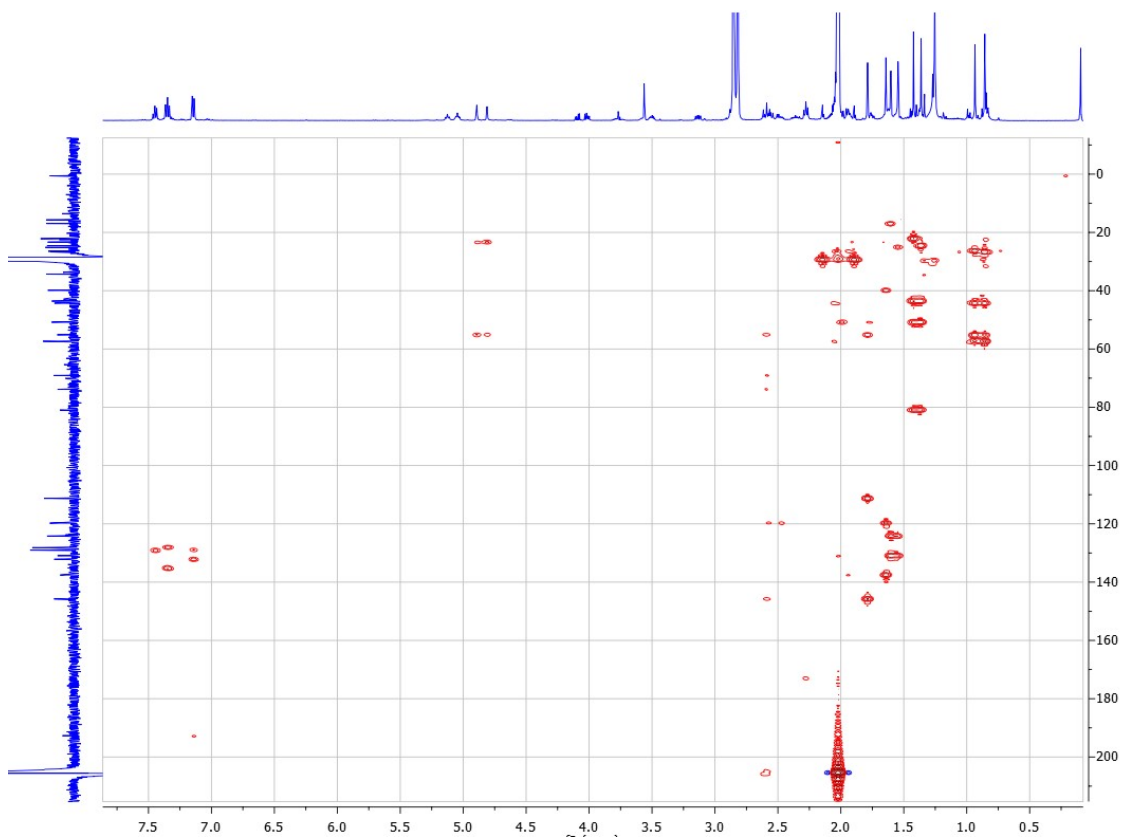


Figure S5H. The HMBC spectrum of **5** in acetone- d_6 .

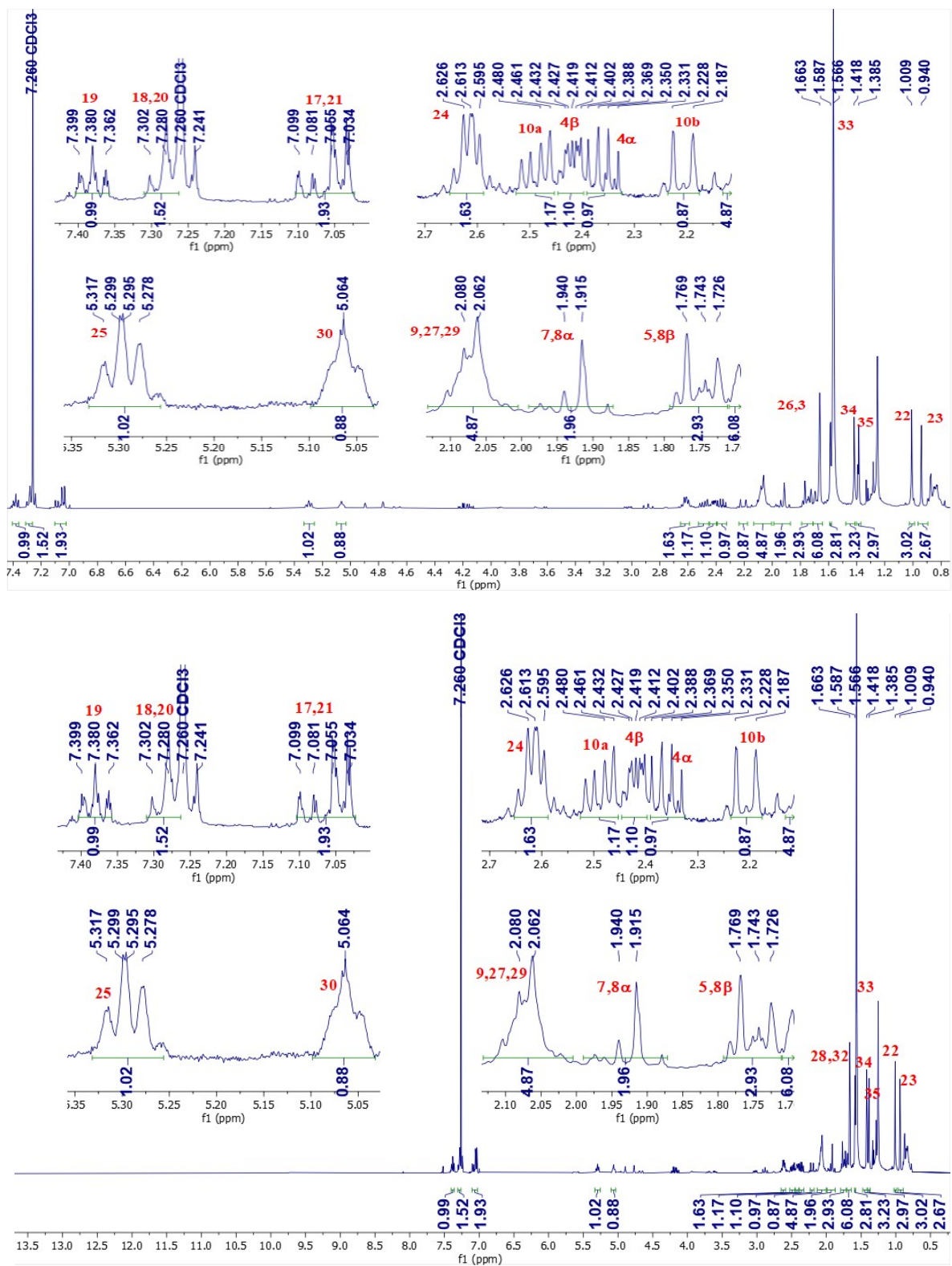


Figure S6A. The ¹H NMR spectrum of 6 in CDCl₃.

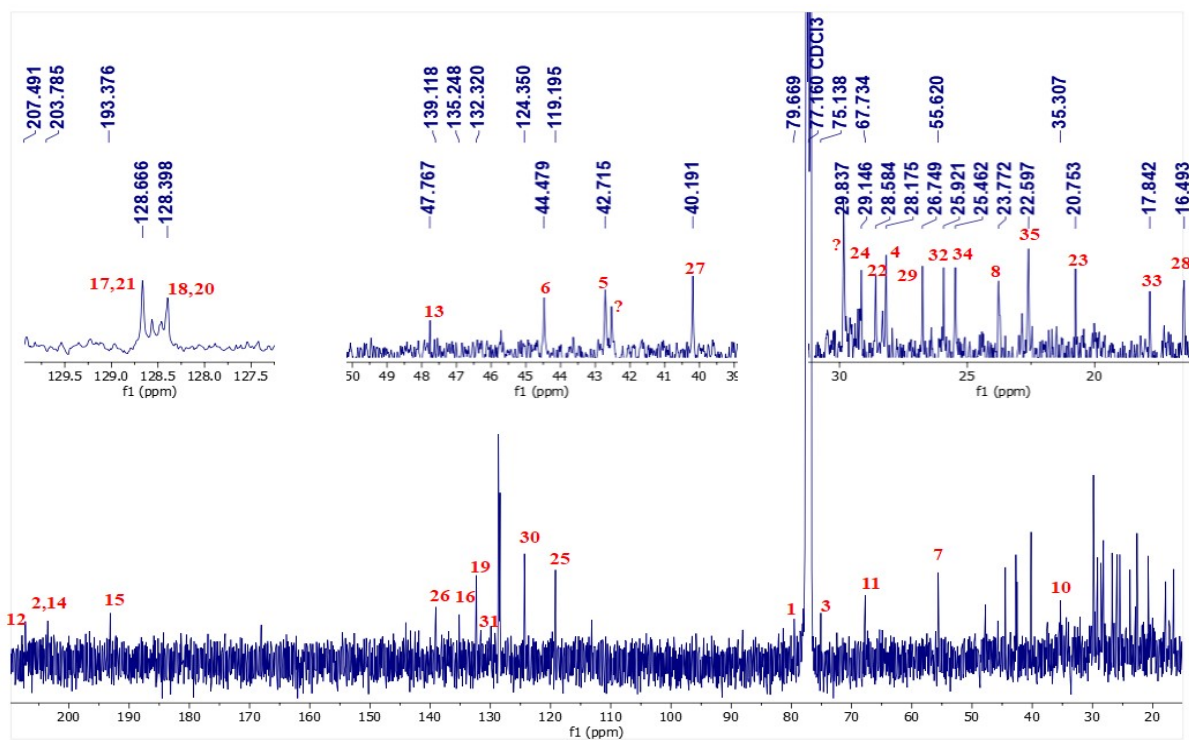


Figure S6B. The ^{13}C NMR spectrum of **6** in CDCl_3 .

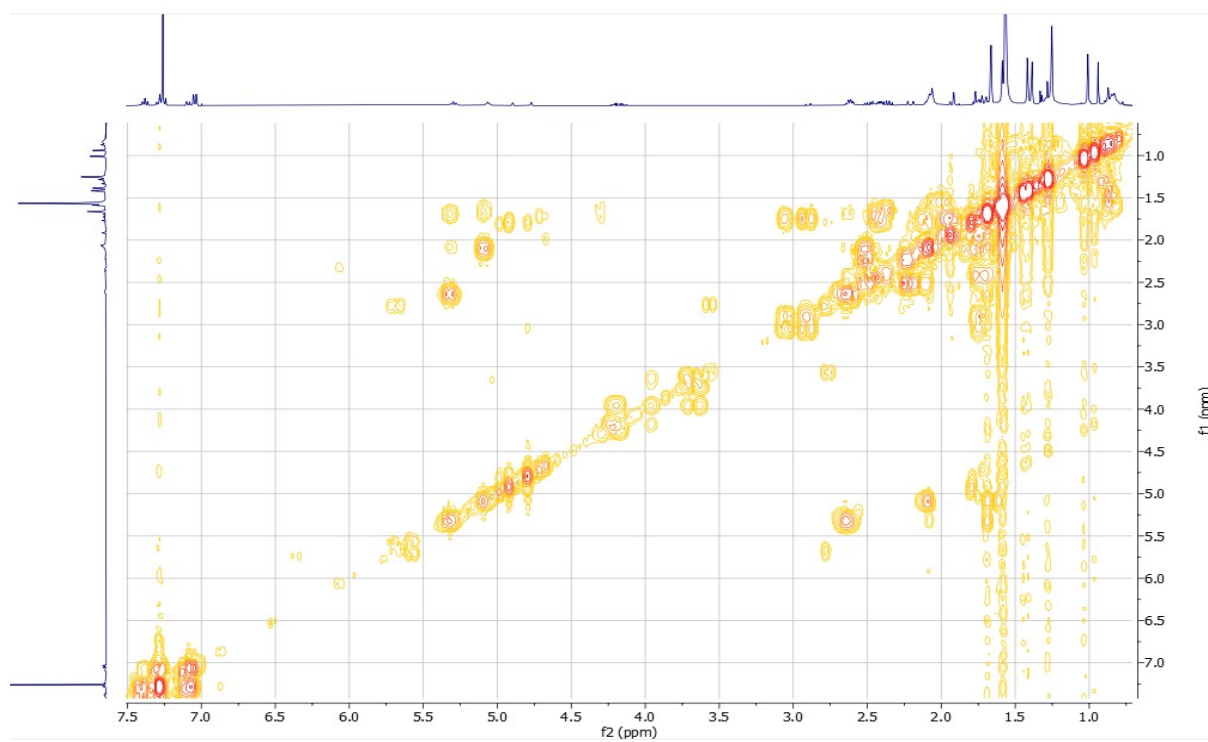


Figure S6C. The COSY spectrum of **6** in CDCl_3 .

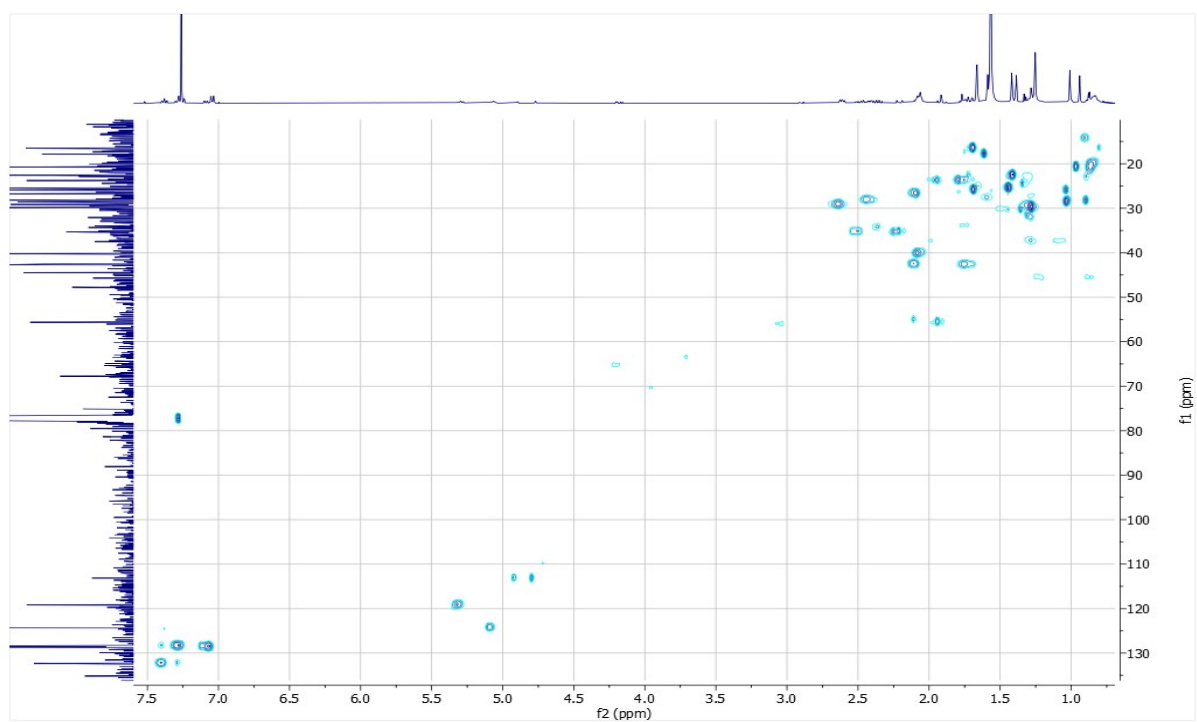


Figure S6D. The HSQC spectrum of **6** in CDCl_3 .

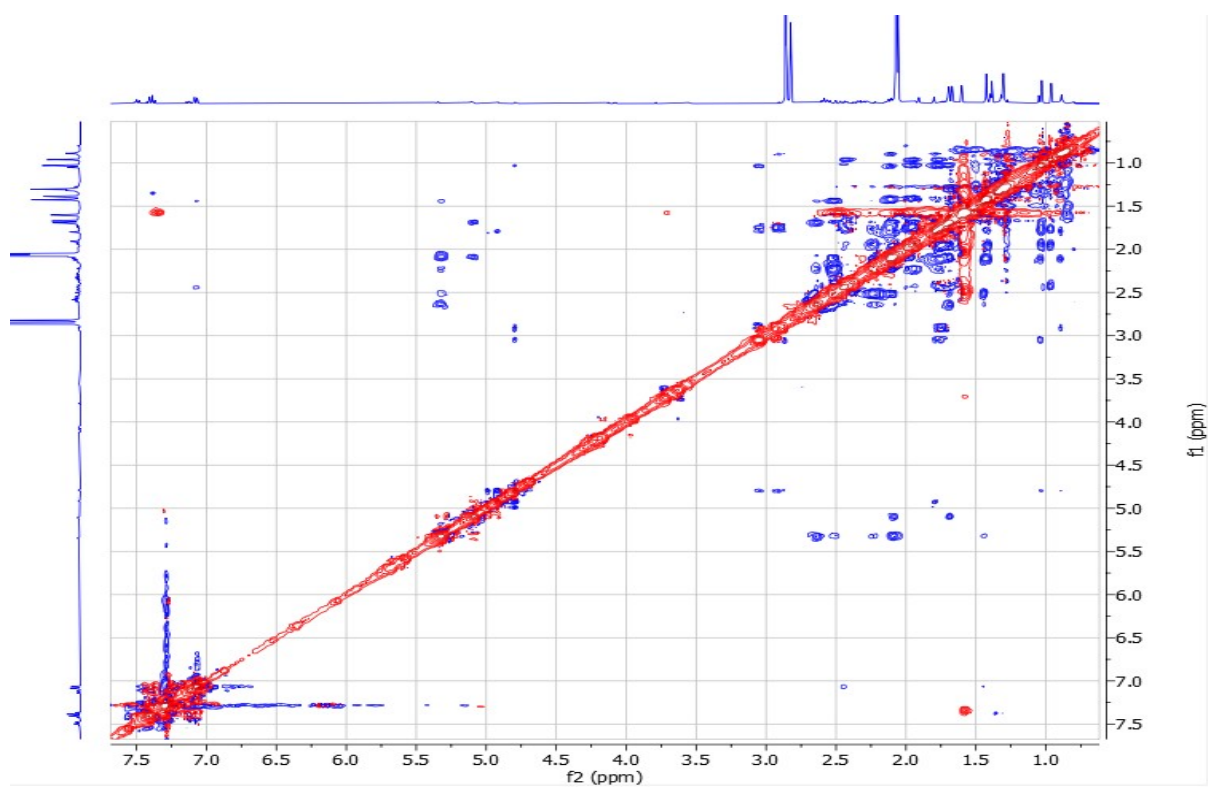


Figure S6E. The NOESY spectrum of **6** in CDCl_3 .

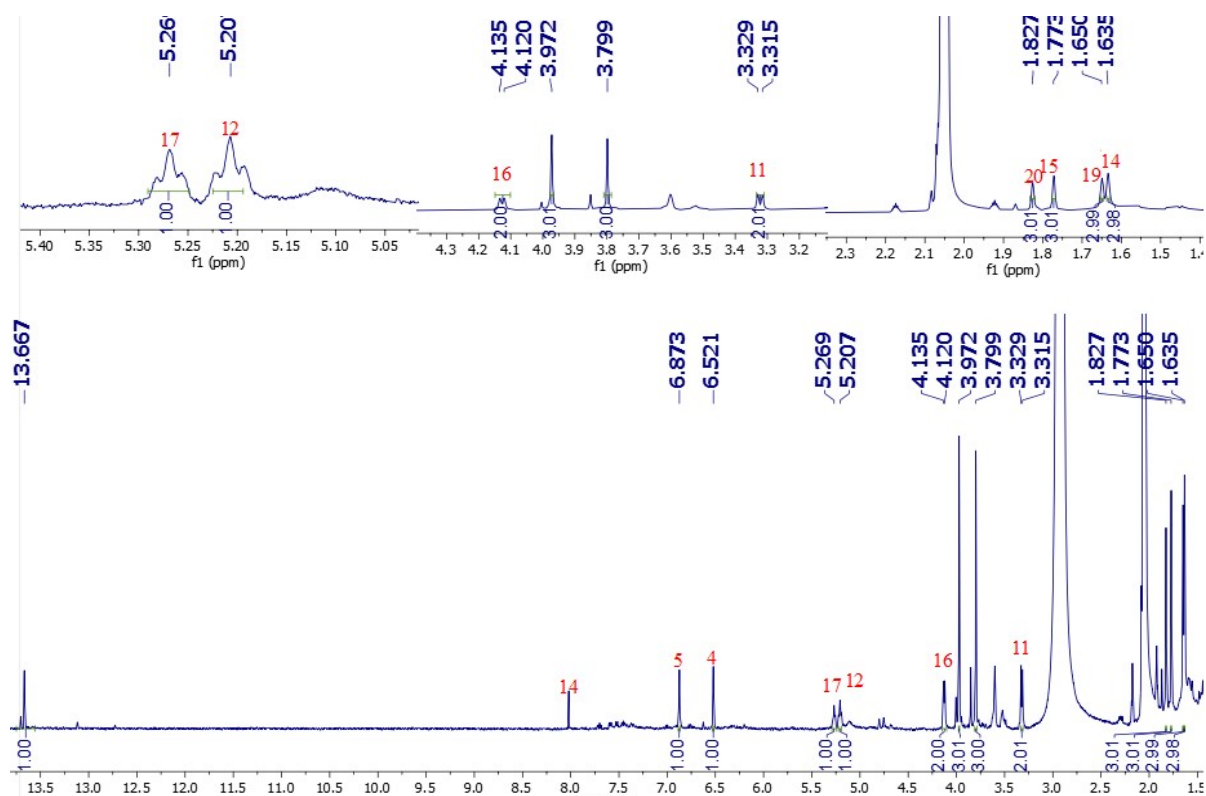


Figure S7A. The ^1H NMR spectrum of **7** in acetone- d_6 .

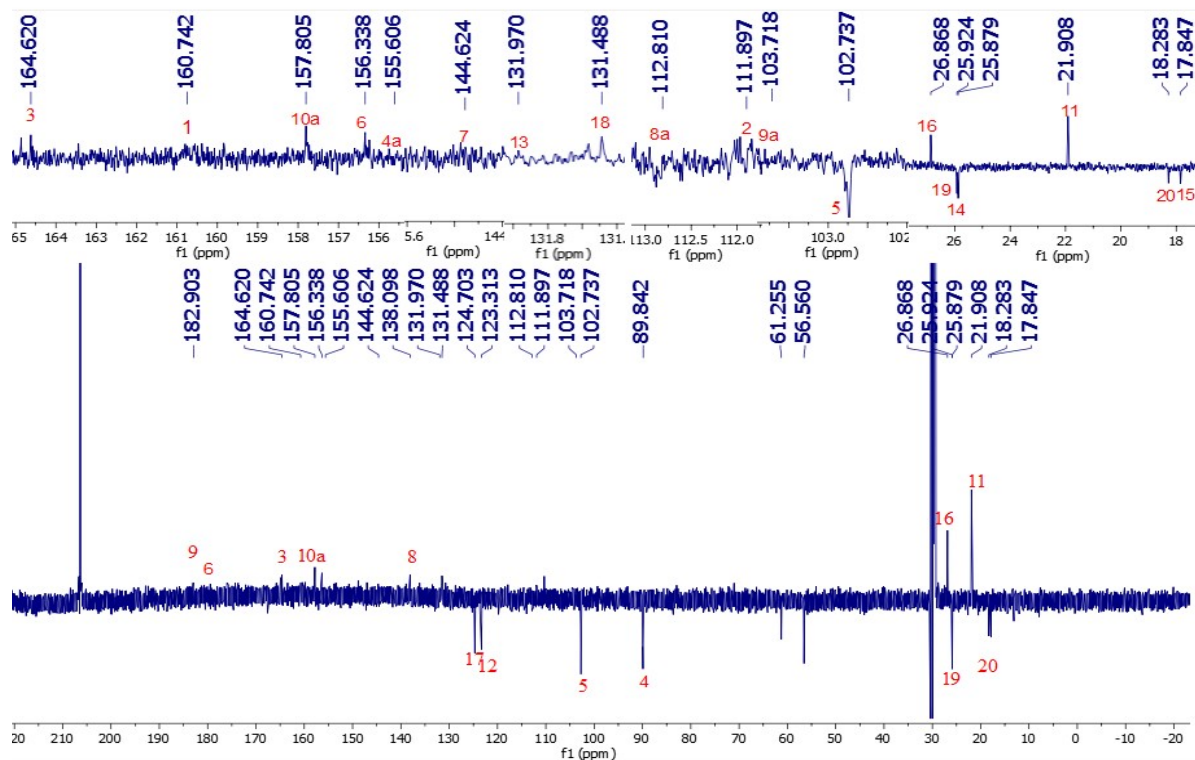


Figure S7B. The ^{13}C NMR spectrum of **7** in acetone- d_6 .

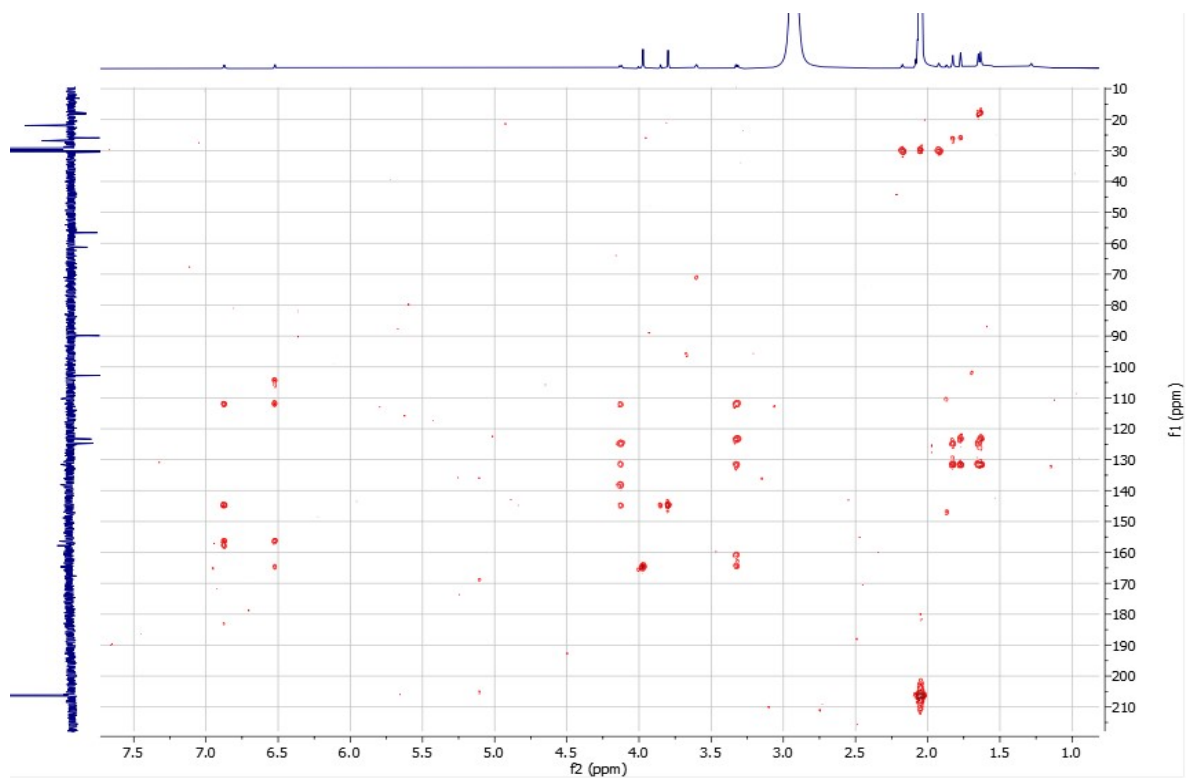
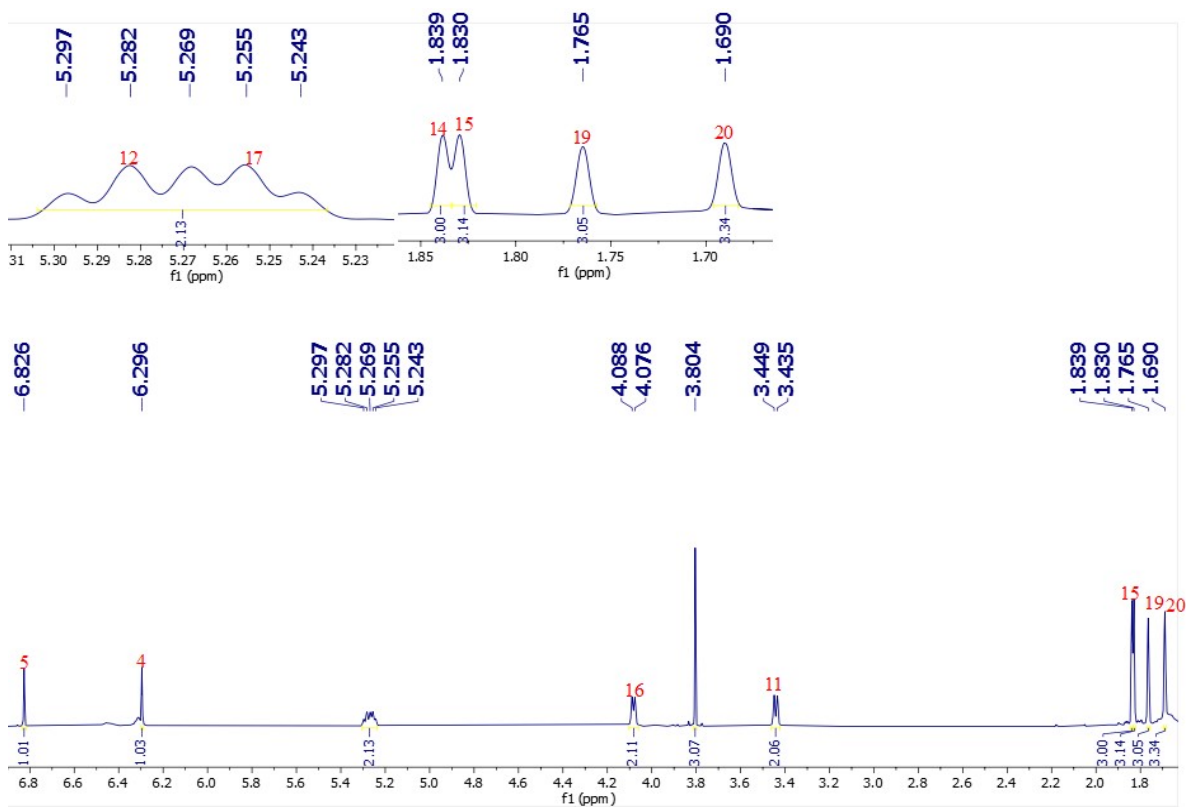


Figure S7C. The HMBC spectrum of **7** in acetone- d_6 .



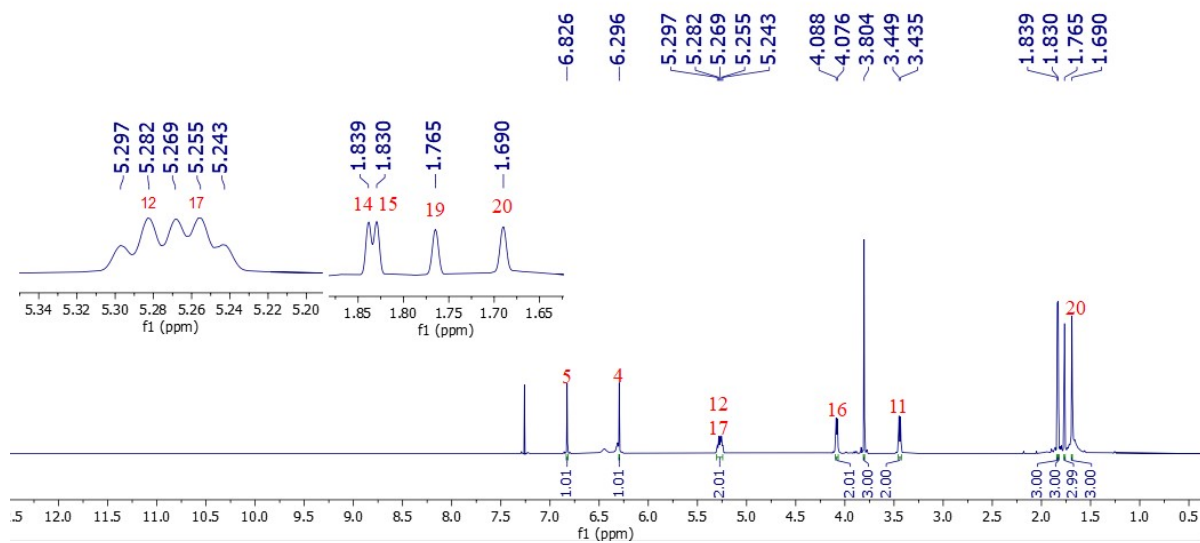


Figure S8A. The ^1H NMR spectrum of **8** in CDCl_3 .

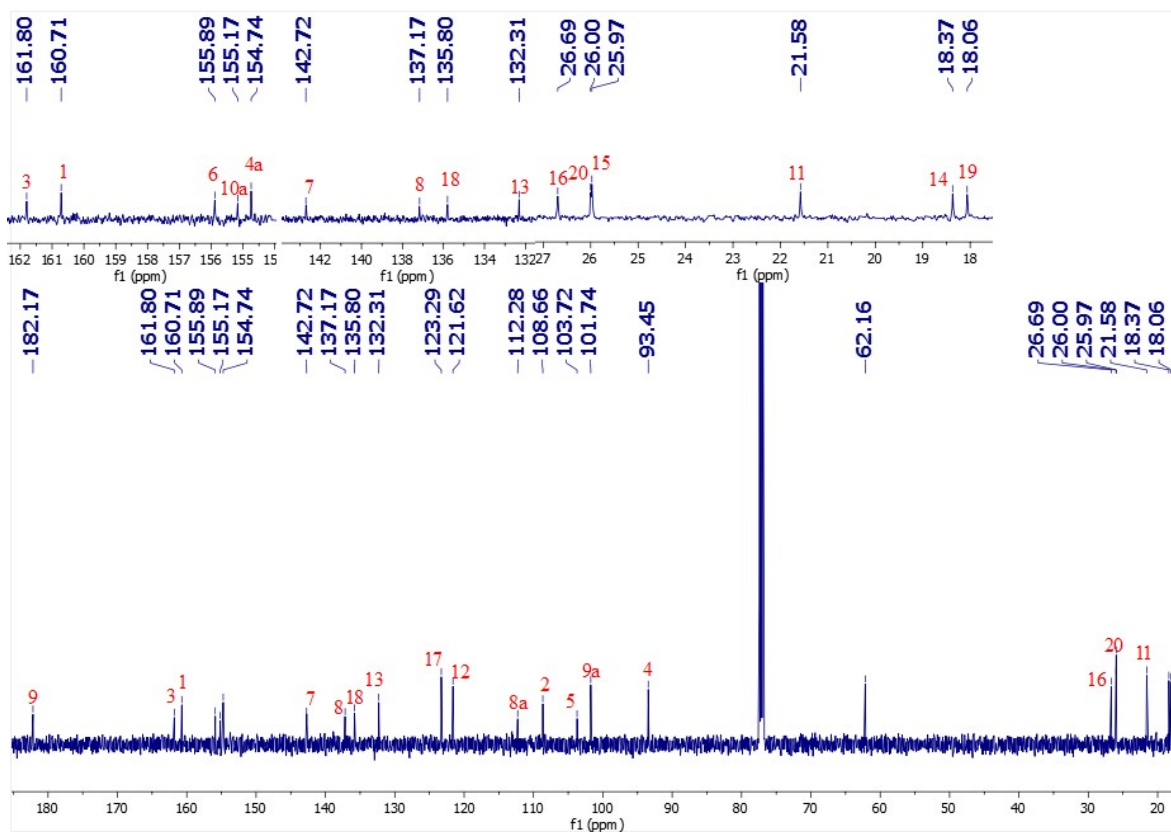


Figure S8B. The ^{13}C NMR spectrum of **8** in CDCl_3 .

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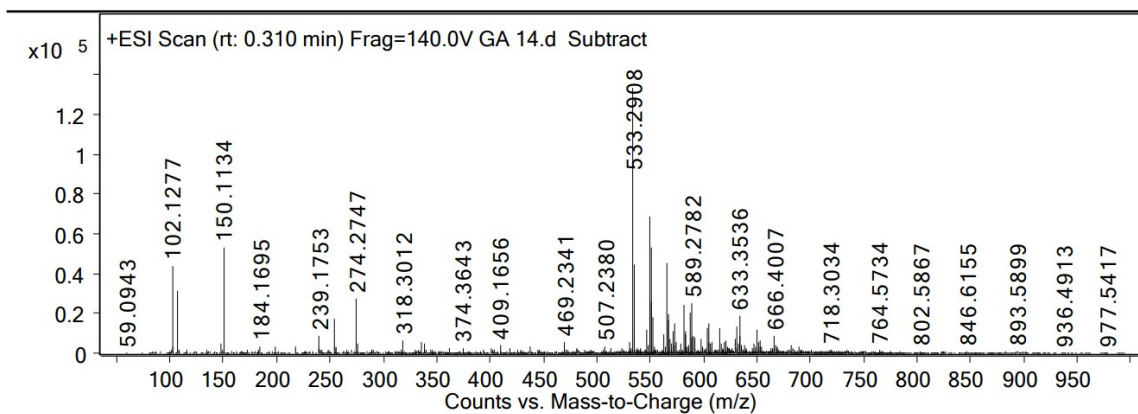


Figure S9A. The HRESIMS spectrum of **9**.

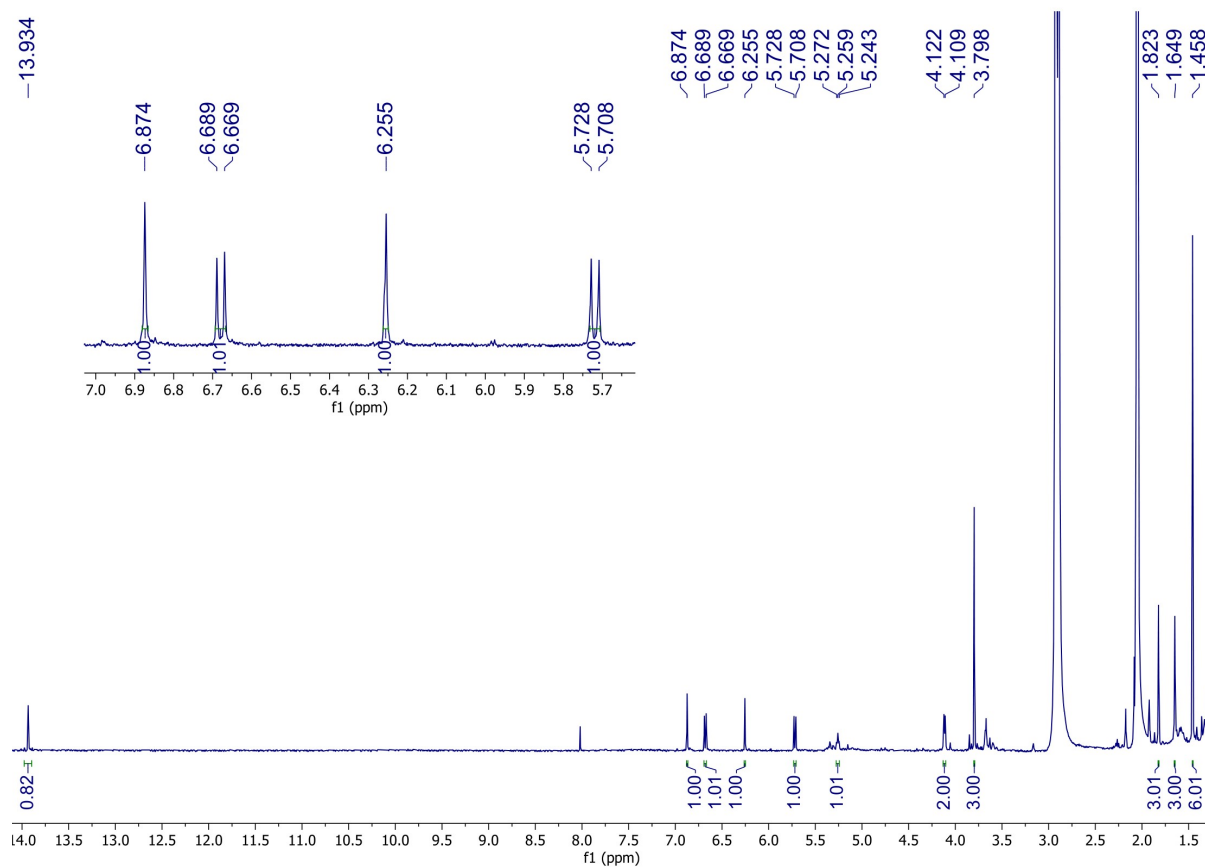


Figure S9B. The ¹H NMR spectrum of **9** in acetone-*d*₆.

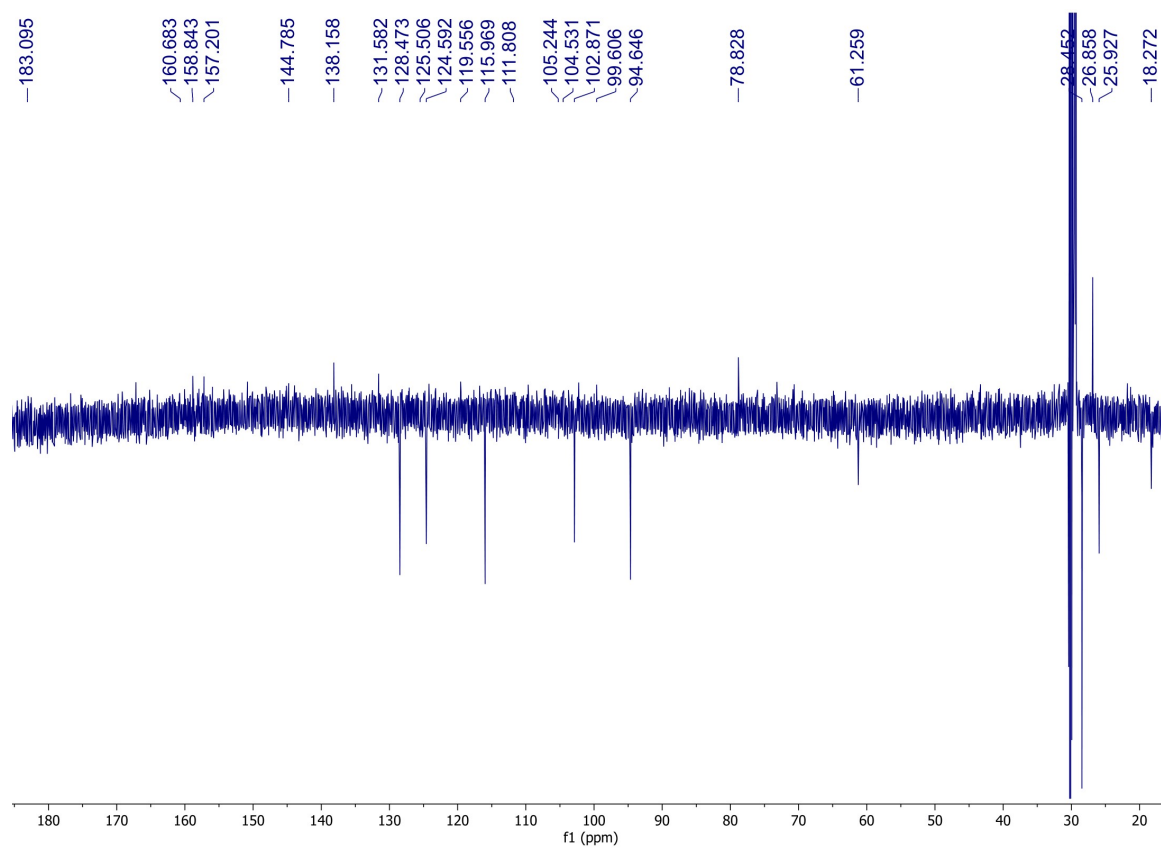


Figure S9C. The JMOD spectrum of **9** in acetone- d_6 .

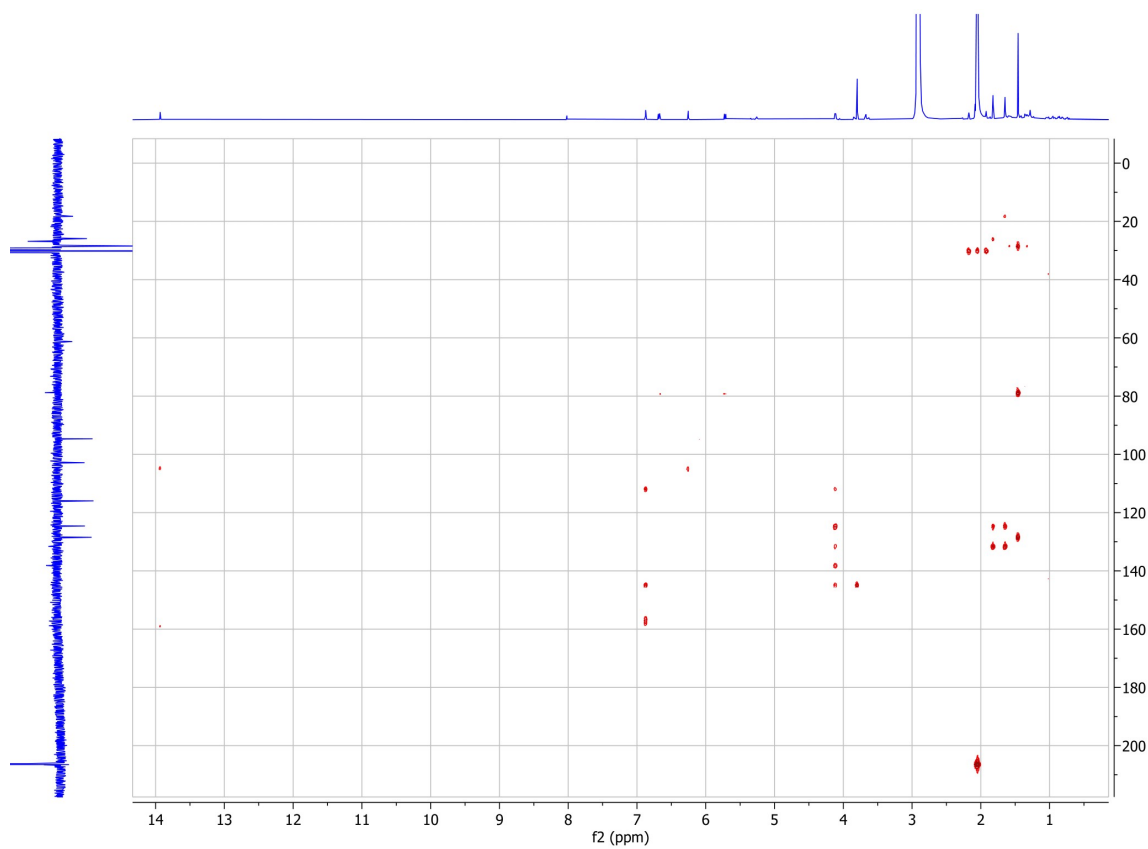
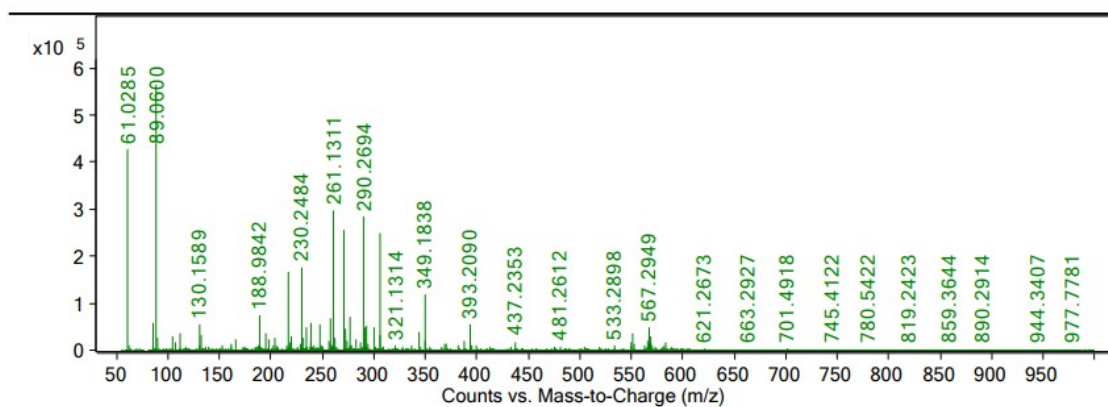


Figure S9D. The HMBC spectrum of **9** in acetone- d_6 .

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494.3509		355.37
494.564		205.74
494.9647		281.74
495.055		371.22
495.1592		580.25
495.1965		994.42
495.2352	1	1494.97
495.2965		602.13
495.4555	2	303.1
495.4863		332.25
495.5369		216.25
495.7124		232.95
495.8749		202.86
495.9645	2	236.01
496.1195		200.75
496.1633		541.26
496.2064		784.31
496.2439	1	759.11
496.307		429.56
496.3364	2	297.27
496.4195		242.72
496.4933		340.88
496.5826		232.44

Figure S10A. The HRESIMS spectrum of 10.

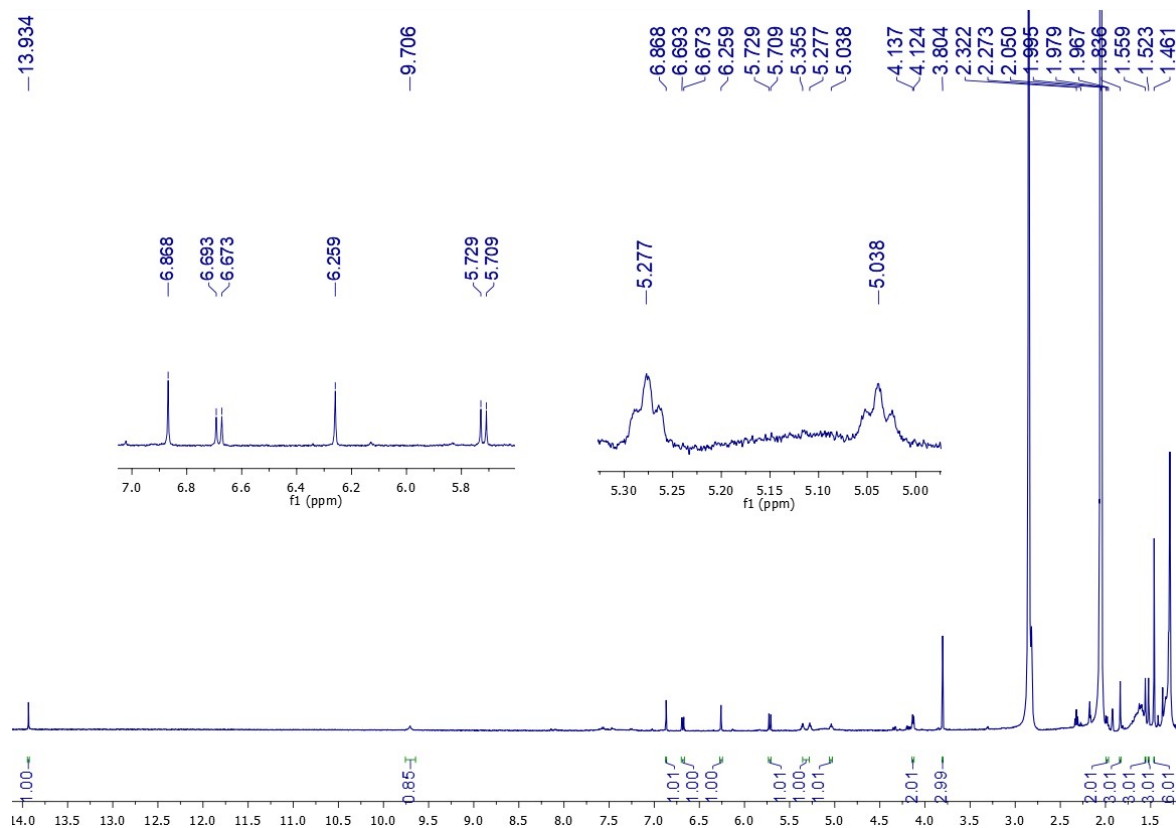


Figure S10B. The ^1H NMR spectrum of **10** in acetone- d_6 .

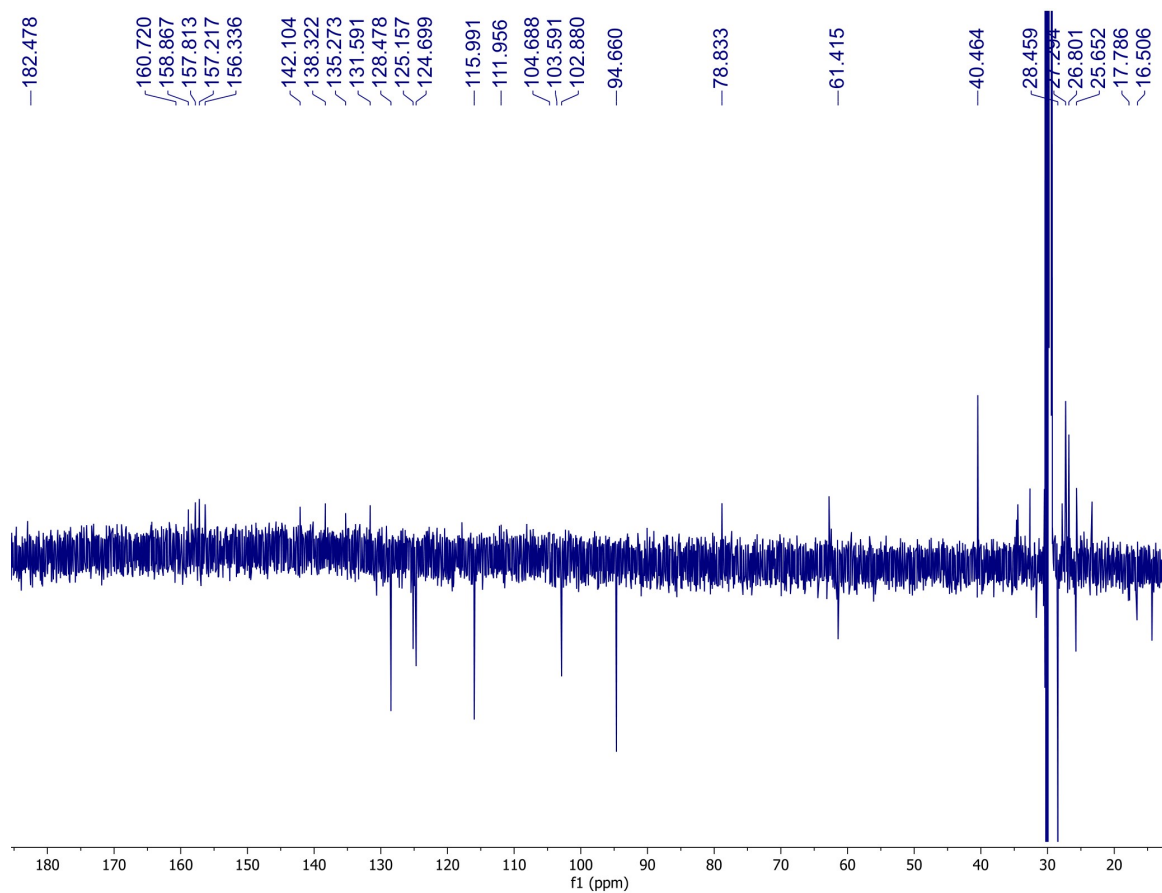


Figure S10C. The JMOD spectrum of **10** in acetone- d_6 .

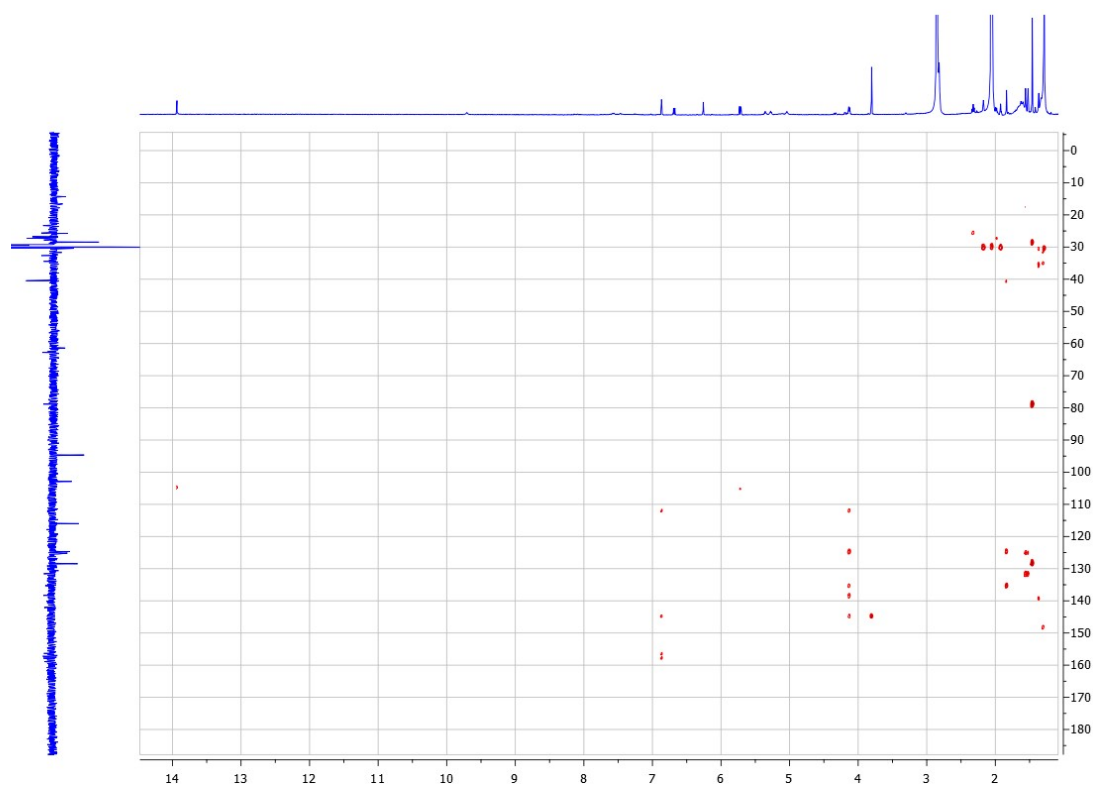


Figure S10D. The HMBC spectrum of **10** in acetone- d_6 .

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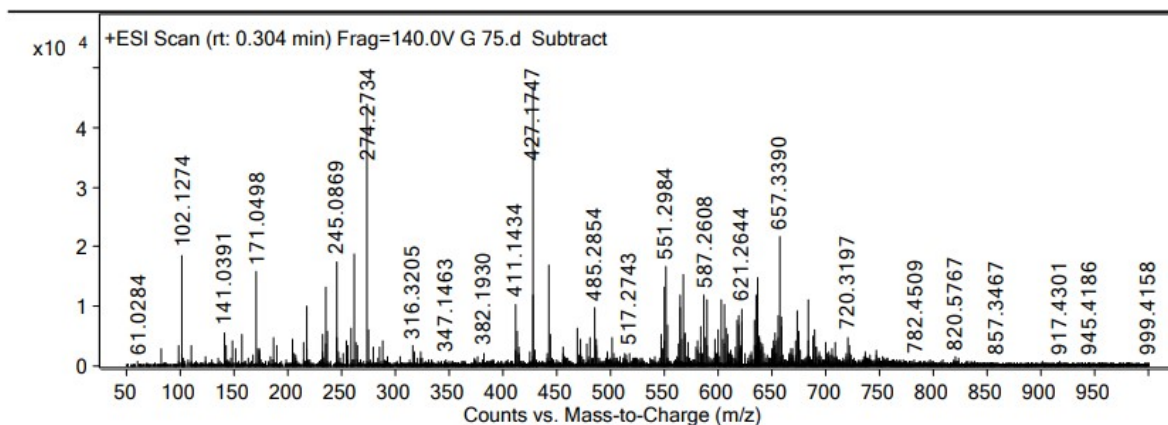
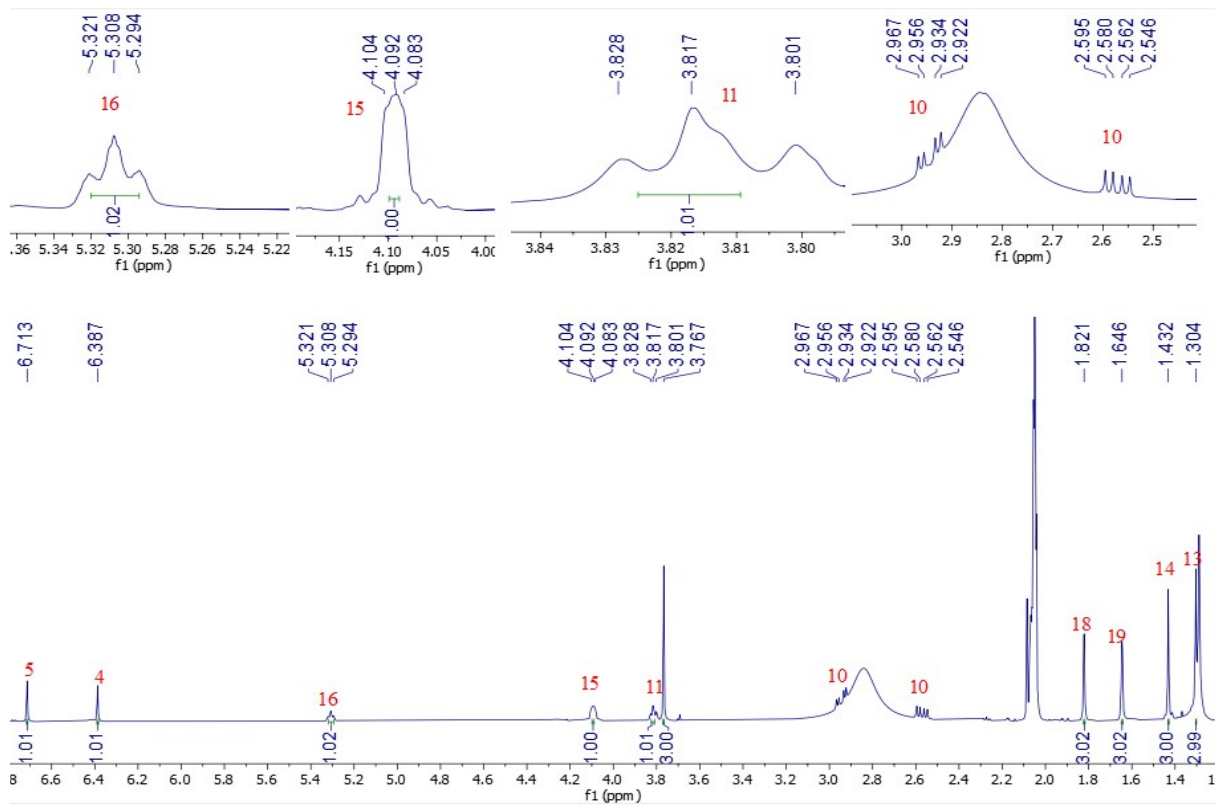


Figure S11A. The HRESIMS spectrum of **11**.



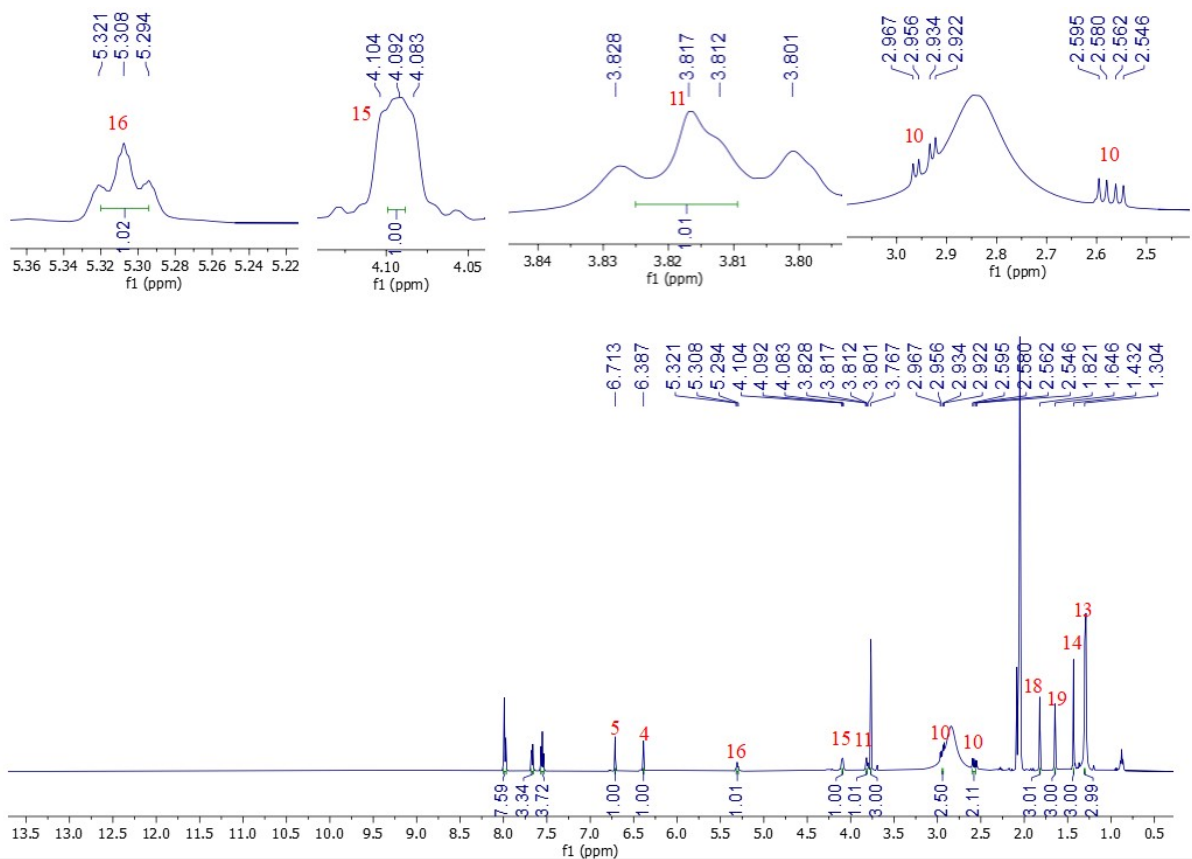


Figure S11B. The ^1H NMR spectrum of **11** in acetone- d_6 .

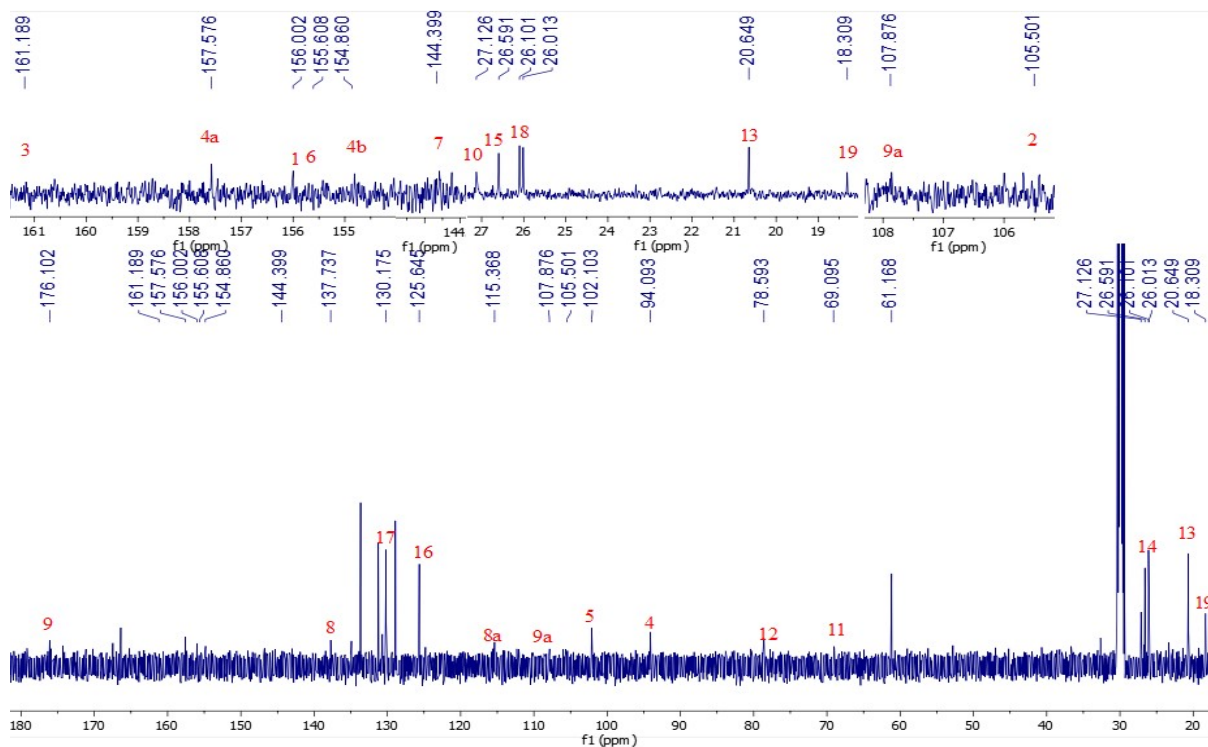


Figure S11C. The ^{13}C NMR spectrum of **11** in acetone- d_6 .

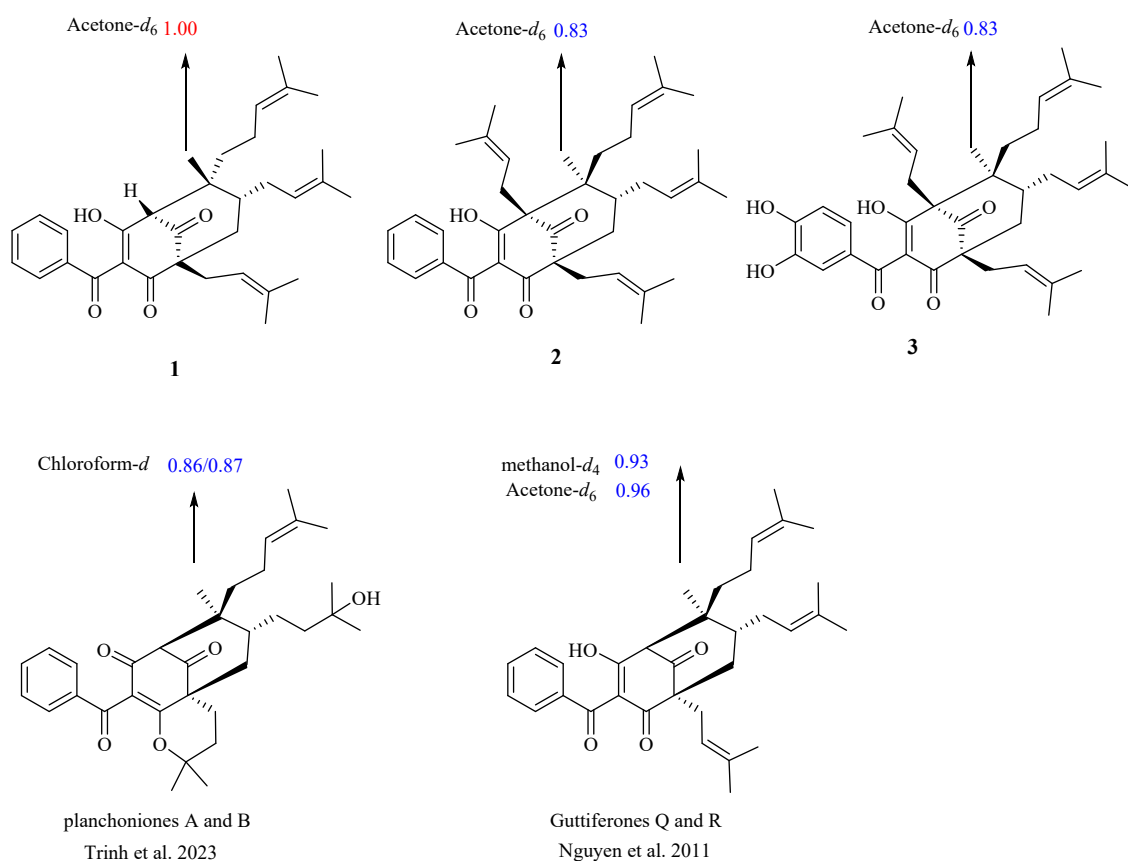


Figure S12. The chemical shifts of the characteristic methyl group of benzoylphloroglucinols 1-3, planchoniones A and B, guttiferones Q and R.

Refs:

X.-T. Yan, Z. An, Y. Huangfu, et al. Polycyclic polyprenylated acylphloroglucinol and phenolic metabolites from the aerial parts of *Hypericum elatoides* and their neuroprotective and anti-neuroinflammatory activities. *Phytochemistry* 2019, 159, 65–74.

H.D. Nguyen, B.T.D. Trinh, L.-H.D. Nguyen. Guttiferones Q-S, cytotoxic polyisoprenylated benzophenones from the pericarp of *Garcinia cochinchinensis*. *Phytochemistry Letters* 2011, 4 (2), 129–133.

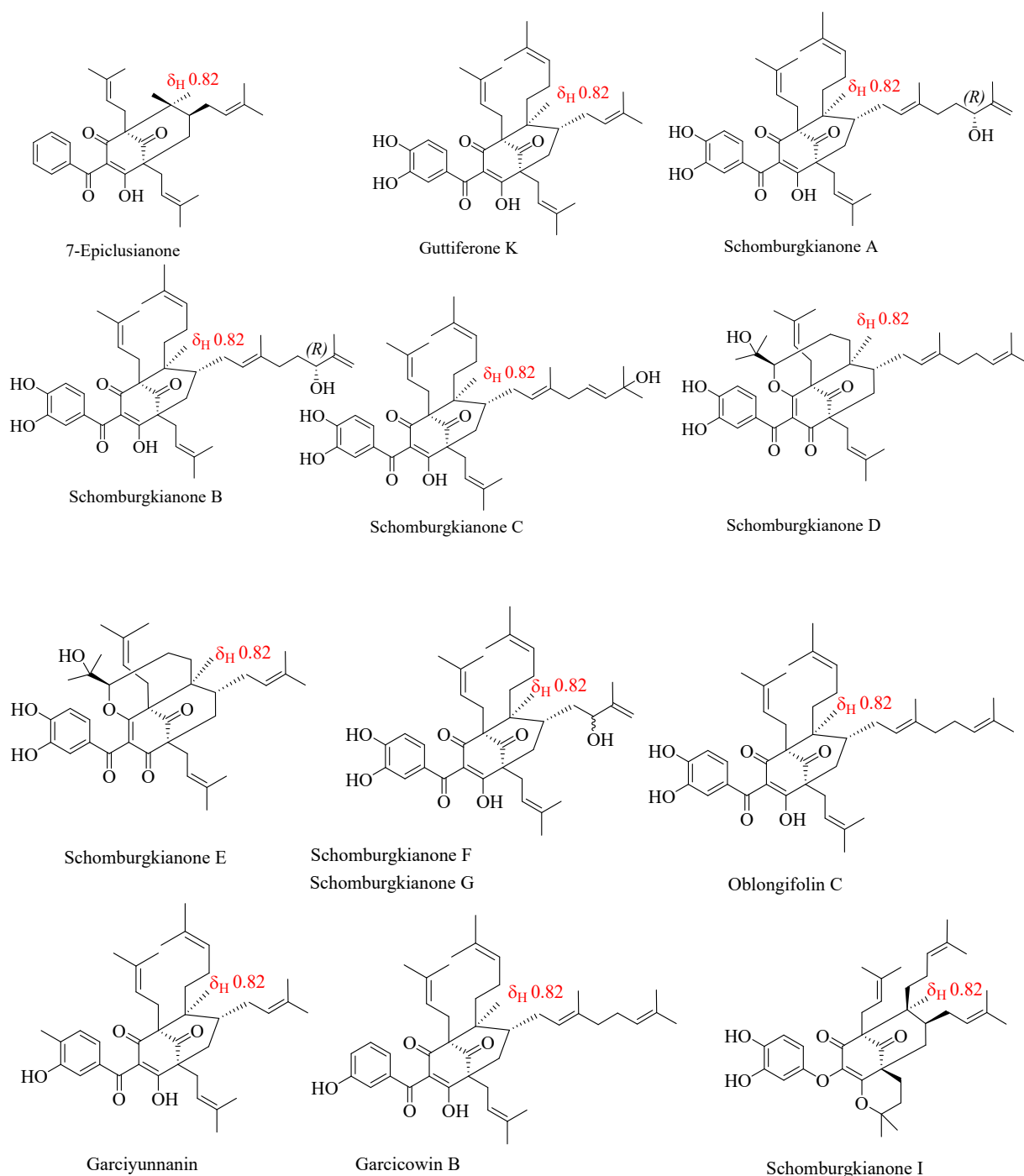


Figure S13. The chemical shifts of the characteristic methyl group of benzoylphloroglucinols from Vietnamese *G. schomburgkiana* fruits.

D.H. Le, K. Nishimura, Y. Takenaka, Y. Mizushima, T. Tanahashi. Polyprenylated Benzoylphloroglucinols with DNA Polymerase Inhibitory Activity from the Fruits of *Garcinia schomburgkiana*. *J. Nat. Prod.* 2016, 79 (7), 1798–1807.

H.T. Nguyen, T.-T. Nguyen, T.-H. Duong, et al. α -Glucosidase Inhibitory and Antimicrobial Benzoylphloroglucinols from *Garcinia schomburgkiana* Fruits: In Vitro and In Silico Studies. *Molecules* 2022, 27 (8), 2574.

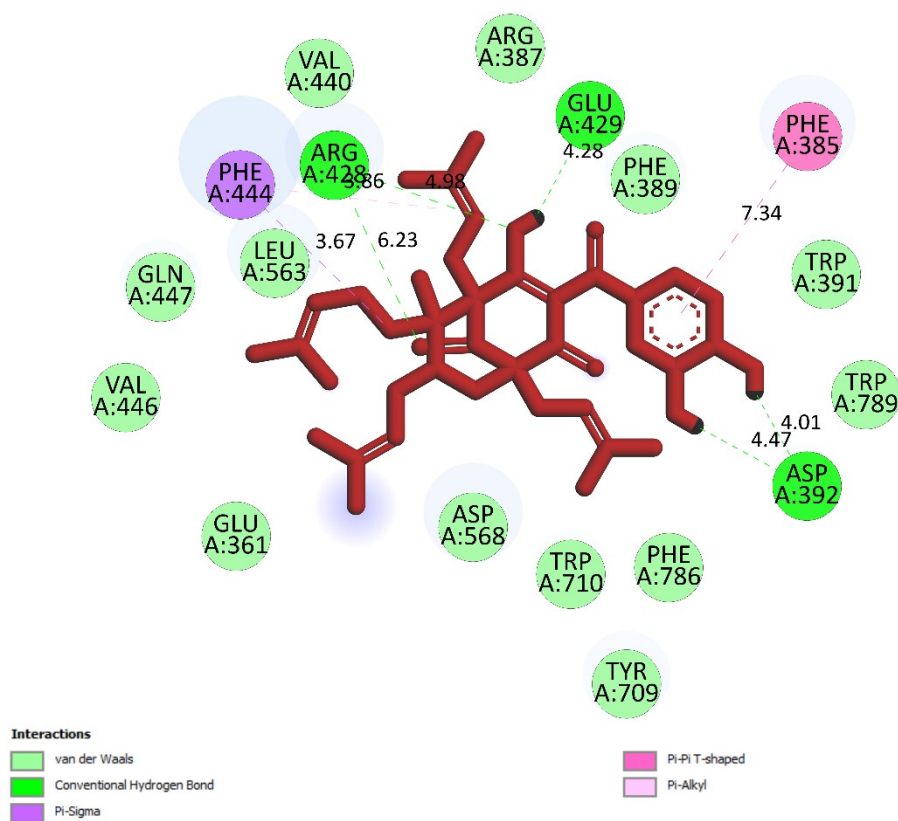


Figure S14. one 2D diagram indicated the significant ligand interactions between pose 82/ compound 3 and residual amino acid on 4J5T enzyme.

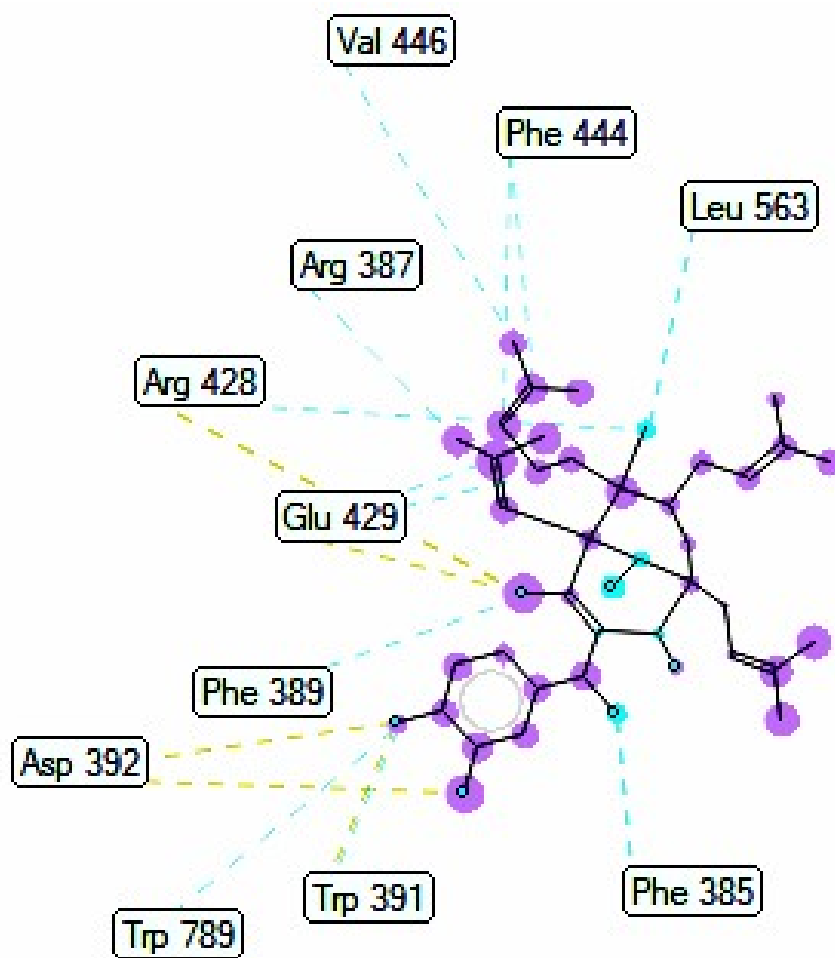


Figure S15. One ligand map indicated the secondary interactions between pose 82/compound 3 and 4J5T enzyme.

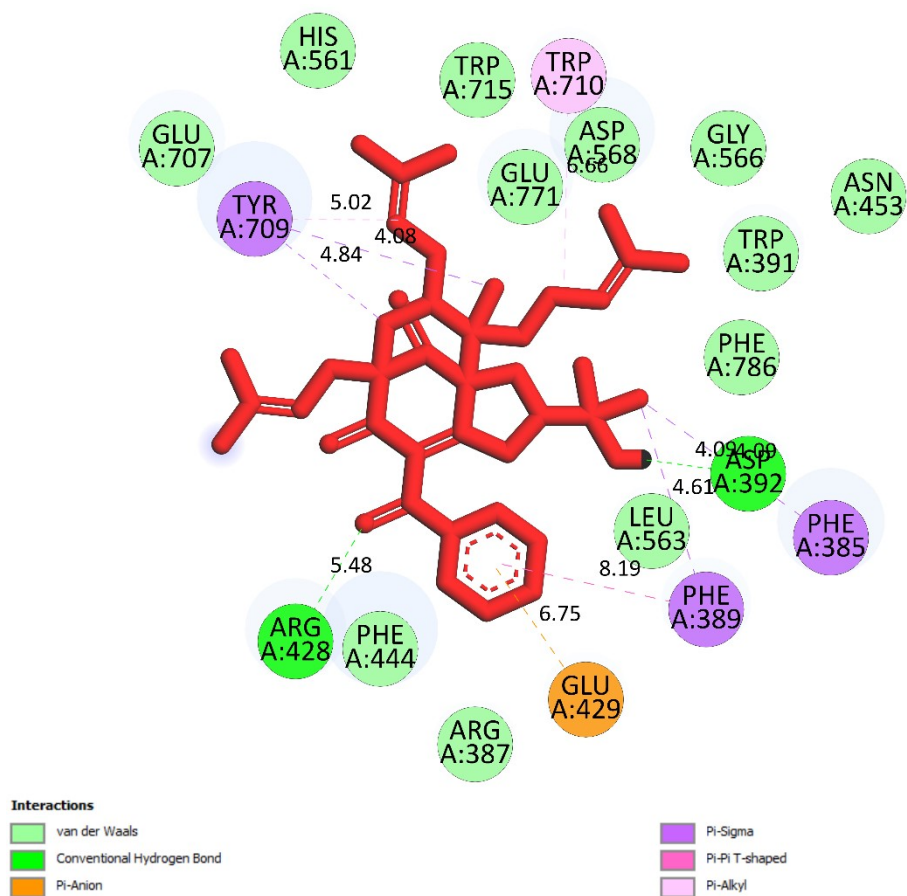


Figure S16. One diagram showed the significant ligand interactions between pose 332/compound 4 and 4J5T enzyme.

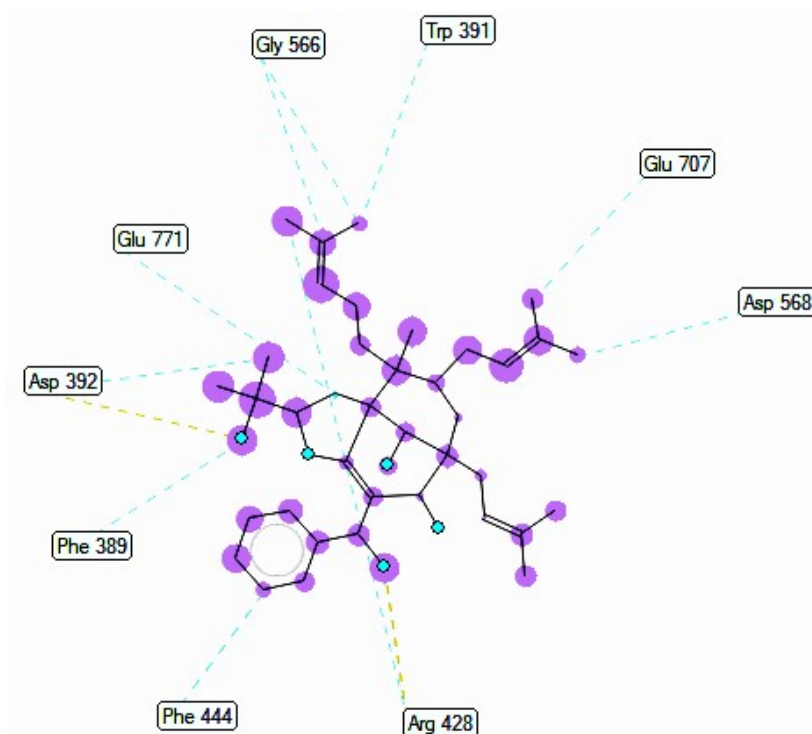


Figure S17. One ligand map showed the secondary interactions between pose 332/compound 4 and 4J5T enzyme.

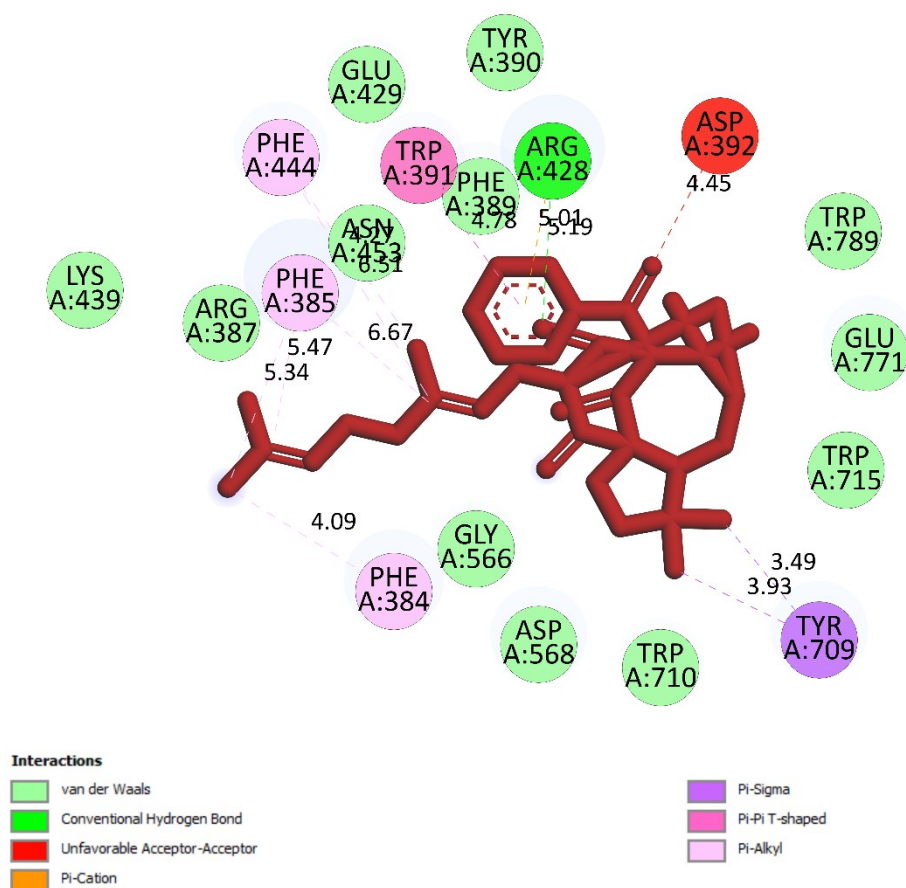


Figure S18. One diagram showed the significant ligand interactions between pose 160/compound 5 and 4J5T enzyme.

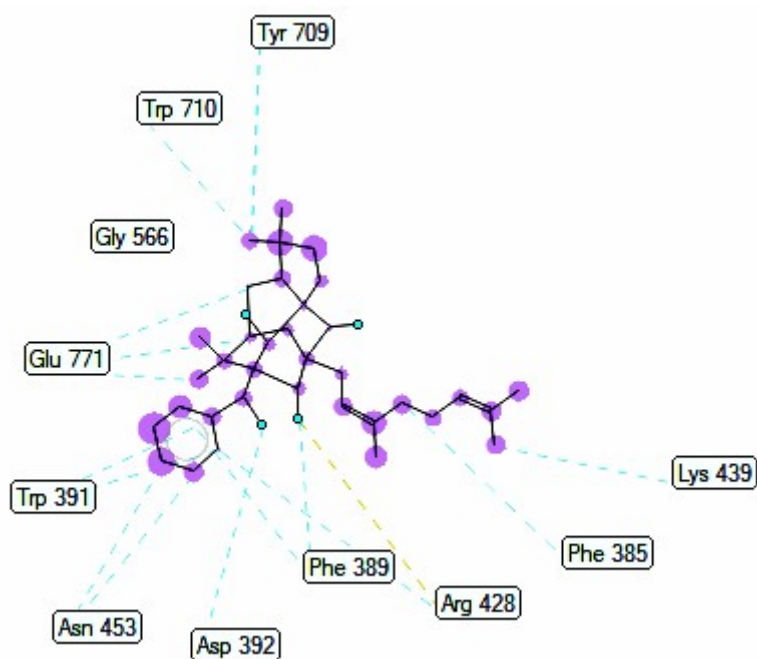


Figure S19. One ligand map showed the secondary interactions between pose 160/compound 5 and 4J5T enzyme.

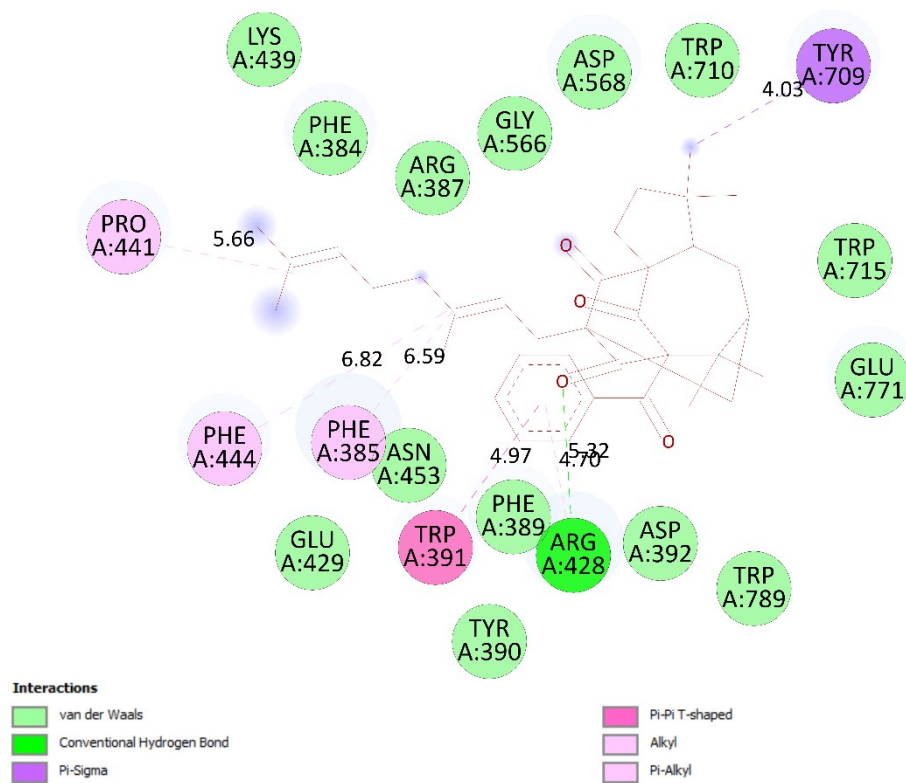


Figure S20. One diagram showed the significant ligand interactions between pose 489/compound 7 and 4J5T enzyme.

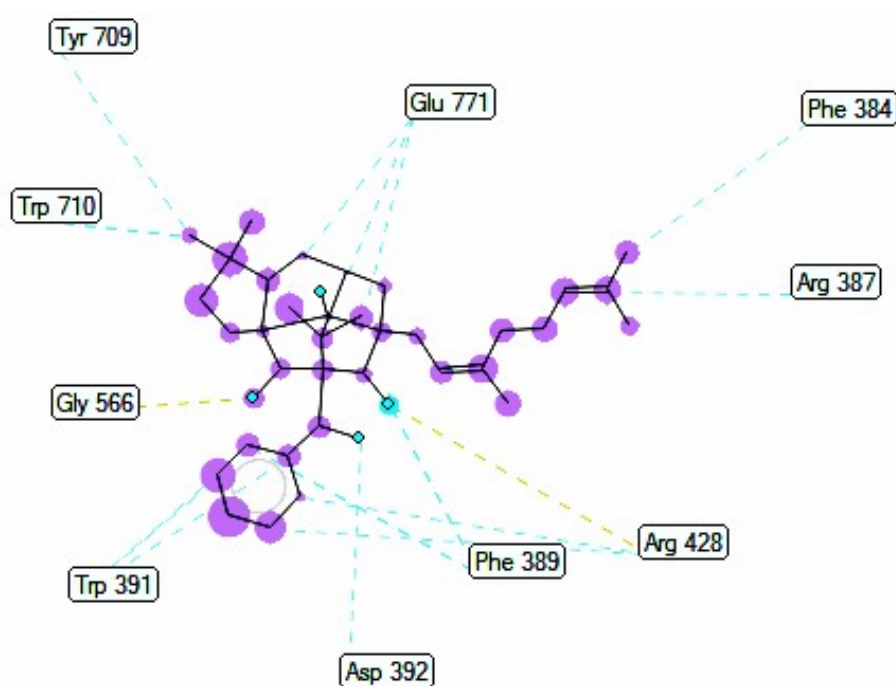


Figure S21. One ligand map showed the secondary interactions between pose 489/compound 7 and 4J5T enzyme.